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Topology Optimization for Highly-efficient Light-trapping Structure in Solar Cell

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1. Abstract
The limitation associated with the low optical absorption remains to be the main technical barrier that constrains the efficiency of thin-film solar cells in energy conversion. Effective design of light-trapping structure is thus critical to increase light absorption in thin-film cells. However, light trapping in thin-film solar cell is a highly complex physical phenomenon governed by several competing physical processes, which imposes a number of challenges to topology optimization. This paper presents a general, yet systematic approach exploiting topology optimization for light-trapping structure designs in solar cells. With simultaneous considerations of all competing physics, we demonstrate that the proposed genetic algorithm (GA) based non-gradient topology optimization (NGTO) approach is robust for achieving highly-efficient designs of slot-waveguide based cell with both low-permittivity and high-permittivity scattering material at single wavelength or over a broad spectrum. A comparative study between the GA based approach and the SIMP based approach for light-trapping structure optimization is made to provide insights into their performances in dealing with different nanophotonic design problems that involve both mild and severe resonances. Even though efforts have been made to improve the regularization scheme of the SIMP based approach, results show that there is a fundamental challenge of using gradient-based topology optimization approach for nanophotoic problems with high nonlinearity.
2. Keywords: Topology Optimization, Light-trapping Structure, Nanophotonic Design, Genetic Algorithm, SIMP

3. Introduction
Thin-film solar cell devices promise an economically viable sustainable energy source due to their potential in low-cost production [1]. However, the significant reduction of active material usage in thin-film solar cells results into a low optical absorption that constrains the device efficiency in energy conversion [2]. Light trapping technology was therefore developed [3, 4] to extend the path-length for light interacting with the active layer, providing solution to the high-efficiency low-cost photovoltaic devices. Since the topological properties of the light-trapping structures play a vital role in determining the governing factors over light absorption in thin-film solar cells, appropriate design of the structure is critical to achieve optimal light-trapping effect, hence the efficient utilization of solar energy.

Recent advances in nanophotonic light trapping [5, 6] open up the new gateway to enhance the optical absorption in solar cells exceeding the so called Yablonovitch Limit [3]. Light trapping in thin-film solar cells is governed by several competing physical processes, including light refraction, deflection, and absorption. Pursuing the optimal structure requires a comprehensive considering of all these competing processes. A wide range of periodic structure have been investigated for light trapping, such as the triangular or pyramid grating [7, 8], nanowires [9], nanoholes [10], nanocone [11], nanoparticles [12], and other nanostructures [13-18]. However, these works are conducted in an ad-hoc fashion that relies on physical intuition to predefine the topology of the light-trapping structure and thus, not capable of handling the topological variation in reaching the optimal design. Therefore, there is a need for an approach that is capable of automatically seeking the optimal topology in delivering highly efficient light-trapping structure.

Topology optimization, originally developed for mechanical structure design problems [19-21] and recently extended to nanophotonic device design problems [22], provides a promising approach for seeking the optimal light-trapping structure for thin-film solar cells. Within the last decade, various high-performance nanophotonic devices designs have been obtained using topology optimization, such as the photonic crystal structure with maximum band-gap [23-25], low-loss photonic waveguide [26], photonic structure for light confinement [27], and the invisible cloak [28]. Nevertheless for the complex nanophotonic light-trapping problem in thin-film cells, limited effort has been made to achieve efficient designs utilizing topology optimization. Miller et al. applied shape optimization approach to seek efficient nanophotonic light trapping structure by decomposing the active/dielectric material interface into Fourier basis functions [29]. However, the optimized interface structure is hard to be realized with existing fabrication techniques. Similarly, Soh et al optimized the active/dielectric material interface using topology optimization approach [30], whereas the design is restricted for total-internal-reflection light-trapping scheme and the results is infeasible for fabrication. Later, Soh et al. obtained a traditional multilayered structure as the optimized design for thin-film silicon solar cells [31]. Instead of directly targeting at the cell absorbing performance, the optimization in their work is formulated to maximize the energy transmitted

into the active layer and limited improvement is observed through their designs.

As topology optimization being applied to different areas, various topology optimization methods have been developed since the seminal work of Bendsøe and Kikuchi [20]. Based on whether gradient information is used in searching a solution, topology optimization methods can be generally categorized into two classes, i.e. nongradient-based topology optimization (NGTO) Methods [32-34] and gradient-based topology optimization (GTO) methods [35-37]. Sigmund made a comprehensive comparison between NGTO and GTO methods from a theoretical perspective [38]. It was noted that GTO methods outperforms NGTO methods in solving conventional mechanical structure optimization problems, but GTO may fail for some special applications, such as certain nanophotonic design problems with numerous local optimums [39]or disjoint design space [40]. However, there is limited research on solving these special problems using topology optimization due to the complexities in physics-based modeling and gradient evaluations. Meanwhile, a comparison between the performances of NGTO and GTO approach in dealing with these non-conventional problems is worthy of investigation.

Considering the aforementioned challenges in efficient light-trapping structure design, we propose a general, yet systematic approach based on topology optimization for achieving highly efficient nanophotonic light-trapping structures with simultaneous consideration of all competing governing factors over light absorption. This approach is robust to the highly nonlinear nature of the nanophotonic light-trapping problem and can be readily applied to solar cell devices with different light-trapping schemes. The optimized design is feasible to fabricate with existing photolithography techniques [41]. While some preliminary results of our method was published [39], an in-depth description and examination of the topology optimization approach is provided in this paper. Both GA based NGTO [39] and SIMP (Solid Isotropic Material with Penalization) [22] based GTO approaches are applied and compared to draw insights into the usefulness of these two methods in solving nanophotonic design problems that involve both mild and severe resonances.

This paper is organized as follows: A brief introduction of light trapping process, the formulation of the light-trapping structure optimization, and the Rigorous Coupled Wave Analysis (RCWA) as the forward analysis model are presented in Section 4. After that the GA based NGTO approach for efficient light-trapping structure design is presented in Section 5 with three demonstrative examples. In Section 6, the SIMP based GTO approach is discussed, which is followed by a comparative study between the two methods for two examples with distinct governing physical characteristics. Conclusion and future work are discussed in the last section.

4. Technical Background

4.1. General Introduction to Light-trapping Process

The theory of light trapping was initially developed for conventional solar cells where the active layer is typically many wavelengths thick, such as conventional silicon solar cells [3]. For a bare solar cell, light will only propagate through the active layer once and the absorption will be smaller with a thinner active layer. However, by texturing the interface between cell and air to direct the light propagation inside the active material, the effect of total internal reflection can be achieved leading to a much longer propagation distance and hence a substantial absorption enhancement. For such light-trapping schemes, random pattern is proved to be optimal with an enhancement on absorption by a factor of $4n^2/\sin^2\theta$ [3], where θ is the angle of the emission cone in the medium surrounding the cell and n denotes the refractive index of the active material. This limit is known as the Yablonovitch limit.

For nanophotonic light-trapping with the thicknesses of active layer comparable to or even smaller than the incident wavelength, certain basic assumptions of the conventional theory are no longer applicable. It has been shown that nanophotonic light-trapping schemes possess the potential to achieve enormous optical absorption enhancement surpassing the Yablonovitch limit [5, 6]. Various nanophotonic light-trapping schemes with sub-wavelength structures have been proposed, including dielectric structures built at that top of the cell [5, 10], photonic crystal structures in the active material itself [42], or metallic nanostructures constructed in the active layer or on the interface between different layer [15, 18]. In these cases, high absorption can be achieved by coupling the incident light into a few distinct modes existing in thin film cells. Random structure is no longer optimal as it couples incident light into continuous modes. Therefore, we aim at a systematic design approach to pursuing the optimal periodic structure designs for nanophotonic light trapping.

4.2. Formulation of the Light-trapping Structure Optimization Problem

In this work, the goal of optimization is to maximize the optical absorption in the thin-film cells. For example, Fig. 1 (a) and (c) present a general structure of a thin-film solar cell model, where the structure on the first layer, i.e. the scattering layer, is the main light-trapping structure to be optimized for maximal absorption in the active layer. The design problem is then recast as the optimization of the material distribution, hence the permittivity distribution $\boldsymbol{\varepsilon}$, within the design space, i.e. the unit cell of a periodic structure shown in the Fig.1 (b).

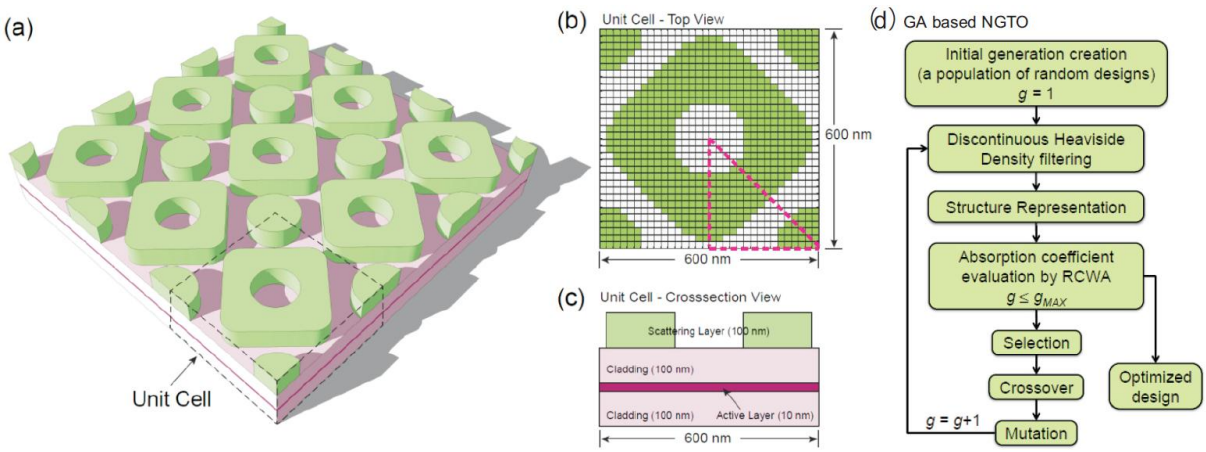

Figure 1: Nanophotonic light-trapping structure optimization model and GA based NGTO framework

The design objective is to optimize the absorbing performance of the thin-film cell, represented by the absorption coefficient *A*. Denoting the absorbed portion of the total incident energy, *A* is the most direct and complete metric judging the absorbing performance of thin-film cells. The formulation of this nanophotonic light-trapping structure optimization problem is shown as Eqn.(1):

$$\max_{\varepsilon} : A(\boldsymbol{\varepsilon}) = \frac{I - R(\boldsymbol{\varepsilon}) - T(\boldsymbol{\varepsilon}) - D(\boldsymbol{\varepsilon})}{I}; \tag{1}$$

where *I* is the incident energy, *R* and *T* is the energy of the zeroth-order reflection and transmission respectively, *D* denotes the deflected energy that considers higher order reflection and transmission, and $\boldsymbol{\varepsilon}$ represents the permittivity distribution. Different from other conventional problems, there is no material resource constraint in this optimization. Nevertheless, the minimum length-scale of the design needs to be controlled for fabrication ease, which can be attained by applying filtering [43].

4.3. Rigorous Coupled Wave Analysis

To evaluate the absorption coefficient *A* in a thin-film solar cell, the Rigorous Coupled Wave Analysis (RCWA) approach [44, 45] is employed. RCWA solves the Maxwell's equations in Fourier space, which is more efficient in both speed and memory than finite difference time domain (FDTD) for dealing with periodic structures (as shown in Fig.1) with plane wave incidence. For a multi-layered photonic system, Fourier expansions in each layer of both the field and the permittivity lead to an algebraic eigenvalue system for each layer. The number of Fourier components considered in the optimization process is 13×13=169. The convergence test was performed on the selection of the diffraction order to ensure the numerical accuracy. As the scattering layer is discretized by a $N_x \times N_y$ mesh, the Fourier components of the permittivity can be calculated using Eqn.(2).

$$\varepsilon(k_x, k_y) = \frac{1}{N_x \times N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \varepsilon(x_i, y_j) e^{-i\cdot(k_x x_i + k_y y_j)}; \tag{2}$$

The electromagnetic fields in each layer are determined by solving a corresponding eigen-problem. The scattering matrix (S matrix) algorithm [46] is then applied on boundary conditions, leading to an S matrix for the whole configuration under investigation. After that, the Poynting theorem is implemented to calculate reflection, transmission, and deflection. The absorption coefficient is evaluated following the law of energy conservation shown in Eqn.(3):

$$\begin{aligned} &A + R + T + D = I; \\ &D = \sum_{n \neq 0} R_n + \sum_{n \neq 0} T_n \end{aligned} \tag{3}$$

5. GA based NGTO for Light-trapping Structure Optimization

5.1. GA based NGTO Method

Genetic Algorithm (GA) is a stochastic search algorithm mimicking the natural evolution process [47, 48]. It has been extended to topology optimization for mechanical structure designs [32, 49]. With the bit-array structure representation, GA provides a natural way for the 0-1 integer programming that is favored by topology optimization problem. Following the idea of survival-of-the-fittest, GA iteratively applies probabilistic operators including selection, crossover, and mutation to search for the optimum; the algorithm is robust to highly nonlinear design problem [47]. In this work, we propose a GA based NGTO approach to optimize the nanophotonic light-trapping structure for thin-film solar cells, as shown in Fig.1 (d). Since the invention of GA method in 1975 [48], a wild array of variants of the original GA has been developed. In our work the standard GA [47] is used. The absorption coefficient value of each structural configuration is evaluated using the RCWA and treated as the fitness value. We use the tournament selection scheme that has been proved to be more favorable than others [50], and the elitism scheme [51] is adopted that the best design within the current generation is preserved to the next generation. The uniform crossover scheme appropriate for 2D topology optimization [25] is used then to perform a structured, yet randomized exchange of topological traits. For the following mutation operation, the design variable value of each element may switch to their opposite phase at a very small probability for potential local refinements that are hard to be achieved through crossover.

As a gradient-free algorithm, GA suffers the curse of limited design dimensionality [38], considering the infinite design dimensionality of topology optimization. However, in designing the nanophotonic light-trapping structure for thin-film solar cells, the design dimensionality is significantly reduced compared with conventional topology optimization problems. First, since the solar cell devices operate under the sunlight containing all polarization angles, symmetrical scattering pattern is preferable for the optimal light-trapping effect [5]. Second, with the consideration of both strong scattering effect and manufacturing feasibility, 10nm resolution is selected as the minimum feature size. In our work, the D_4 symmetry constraint is imposed on the 600nm×600nm unit cell discretized with a 64×64 mesh. In this case, the design space is reduced to the triangular area denoted in Fig.1 (b) to facilitate the GA based NGTO in seeking the effective light-trapping structure feasible for fabrication.

As a stochastic algorithm, GA renders the issues of numerical instabilities [52] and disconnected features in using conventional topology optimization to mechanical structure designs [32]. A discontinuous Heaviside density filter is applied in this work to alleviate the numerical instabilities in GA based NGTO. The gradient-free characteristic of GA and the absence of volume constraint enable the use of the true Heavside step function in the filter. The design variables $\mathbf{x}$ valued either 0 or 1 are first mapped onto the element space by computing the distance-weighted average following the conventional density filtering process [43]. After that, a true Heaviside step function with the threshold value of 0.5 is applied to achieve a pure 0-1 design. It should be noted that the element pseudo density $\boldsymbol{\rho}$ through the discontinuous Heaviside density filter carries the physical meaning [43]. The structure evaluated by the RCWA is the permittivity distribution $\boldsymbol{\varepsilon}$ determined by ρ, whereas the GA operators, i.e. selection, crossover and mutation, are performed on the designs represented by $\mathbf{x}$. In this way, the filtering process not only prevents the numerical instabilities associated with the GA based NGTO, but controls the minimum feature size for the fabrication ease as well. For the aforementioned feature connectivity that requires careful handling in conventional problems using GA based NGTO [32], the disconnected features are usually favorable in the nanophotonic devices optimization [23, 40].

With the GA based NGTO framework determined, a proper set of control parameter in GA is critical for a competent optimization. The 3-step methodology [51] is followed in this work to determine the values of GA parameters. The population size N_p, i.e. the number of designs within one GA generation, is selected to be $2\times N$ (N is the number of design variables). The total number of evolving generation N_g is set *as* $1.4\times N_p$ and the elitism scheme [51] is adopted to preserve the best design within the present generation to the next generation. The parameter s for the tournament selection scheme, denoting the number of candidate designs in tournament selection, is chosen to be 2. The values of crossover probability P_c and mutation probability P_m are thus chosen to be $(s\text{-}1)/s$ and $1/N_p$, respectively.

5.2. Nanophotonic Light-trapping Structure Optimization Results using GA based NGTO

The proposed GA based NGTO approach for nanophotonic light-trapping design is first applied to the slot-waveguide based thin-film solar cell shown in Fig.1 (c). Two different materials for the scattering layer are tested as two examples with differing physical characteristics. In these examples, a normal incidence at $\pi/4$ polarization angle is applied and a D_4 symmetry constraint is imposed on the unit cell.

Example 1: Slot Waveguide based Solar Cell with Low-permittivity Scattering Material

Recently, a promising nanophotonic light-trapping scheme [5] is investigated utilizing the so called slot-waveguide effect [53]. A slot waveguide is an optical waveguide that can confine light in a sub-wavelength region of lower permittivity bounded by higher permittivity regions. By careful design of the light-trapping structure for the slot waveguide, the light absorption can be greatly increased with an enhancement factor beyond

the Yablonovitch Limit. Therefore, we use this example to demonstrate the GA based NGTO approach in achieving highly-efficient light-trapping structure. As shown in Fig.1 (c), the test structure of slot-waveguide based cell consists of an ultrathin P3HT:PCBM active layer of 10nm thickness, which is sandwiched between two 100 nm thick cladding layers made of high index gallium phosphide (GaP), and a nano-structured light scattering layer on top. The scattering layer couples the incident sunlight to the corresponding slot waveguide modes by matching the differences in wave vectors [54]. The optical field will then be confined within the active layer by the virtue of the slot-waveguide effect. In this process, the light-trapping structure to be designed, i.e. the scattering layer, plays a critical role in balancing the competing process of light reflection at the front and the light diffraction for effective coupling to the slot waveguide modes.

In this example, to simplify a design problem associated with multiple governing factors, which often results in a complex solution space with numerous local optima, the low-permittivity polymer material (ε=2.89) was used to construct the scattering layer. Under the effective medium approximation, the effective refractive index of the scattering layer is determined by averaging the dielectric and air regions, ranging from 1 to 2.89, which is much smaller than that of the cladding layer (ε=12.75). Therefore, the reflection at the top surface due to the impedance mismatch [55] becomes insensitive to the variation of the scattering layer while leaving the diffraction and the subsequent mode coupling being the dominating factors in the optimization process.

A 32×32 coarse mesh is applied for this test, which is adequate in delivering efficient designs based on tests. Considering the coarse mesh and the simplified physics due to the choice of low-permittivity material in the scattering layer, no filtering is applied. Starting from the initial generation composed of random designs, the GA based NGTOs converge to the optimal scattering patterns maximizing the absorption for incidence at λ = 400nm, 500nm and 600nm, as shown in Figs.2 (a), (b) and (c), respectively. The optimized unit cell is denoted with the dashed square window, and the whole pattern represents a 3×3 cells array. The convergence is achieved within 120 generations as shown in Figs.2 (d), (e) and (f), where the significant enhancement on the light absorption through the optimization can be observed. Absorption coefficients of the optimized patterns are summarized in the second row of Table 1. It should be noted that the optimized absorption for λ=500nm is low compared with other incident wavelengths due to the deconstructive interference in this multi-layered solar cell system[39]. The optimized scattering structures with periodic patterns imply the effective coupling of incident plane wave to the discrete photonic modes, which can also be proved using the Fourier analysis[39].

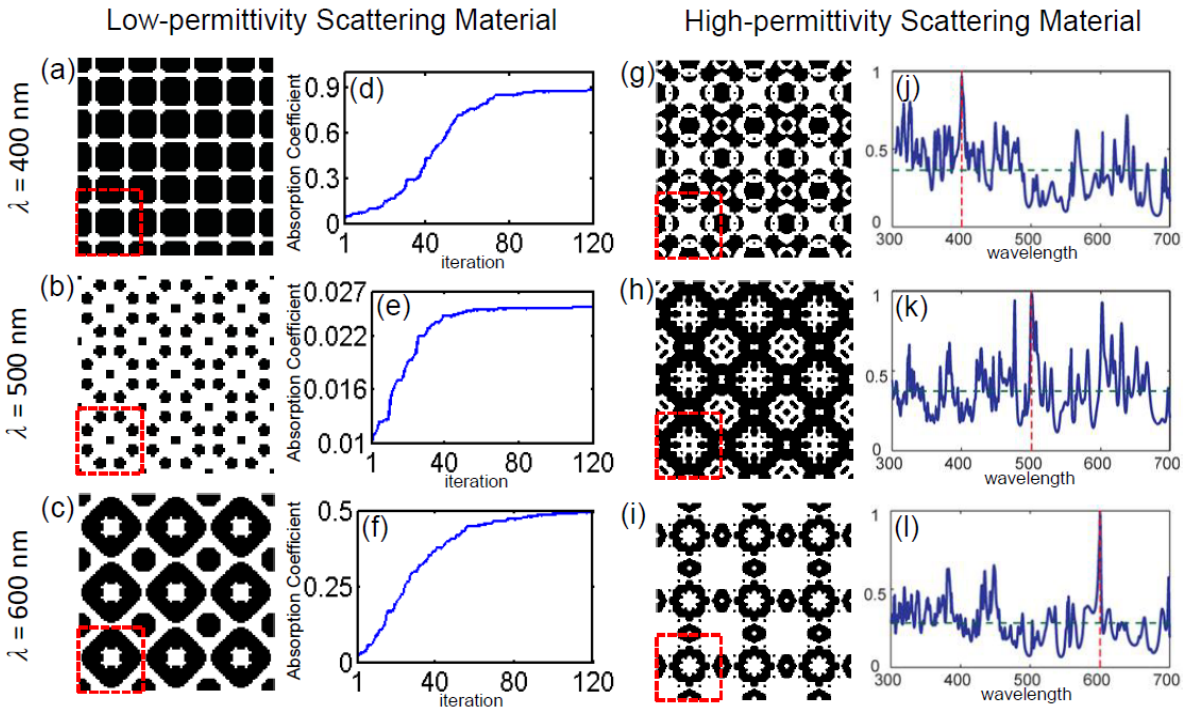

Figure 2: Optimized results using GA based NGTO

Table 1: Absorption Coefficient of Optimized Design using GA based NGTO

Targeting Wavelength	λ = 400 nm	λ = 500 nm	λ = 600 nm
Low-permittivity Scattering Material	0.890	0.026	0.499
High-permittivity Scattering Material	0.964	0.985	0.991

Example 2: Slot Waveguide based Solar Cell with High-permittivity Scattering Material

In this example, the dielectric material in scattering layer is replaced with high index dielectric (GaP), which is identical to the material used for the cladding layer. While the overall absorbing performance can be improved, the use of high-index dielectric material in the scattering layer leads to a more complicated optimization problem with multiple governing factors in effect. In this case, the scattering layer with proper spatial filling ratio of the dielectric material determines the reflection of the incident light due to the impedance mismatch and the simultaneous diffraction to the targeted slot waveguide modes. Due to the fact that the geometry change on the scattering layer has a significant influence on both diffraction and reflection, those two competing processes need to be addressed simultaneously during the design process. Competition between these two factors brings forth a large number of local optimums and the stronger scattering effect leads to severe physical resonances, which unfortunately increases the complexity of solution space. Moreover, stochastic search algorithms are vulnerable to "structural noise" in that checkerboard patterns and redundant small scale features appear during optimization iterations and in the final results [32]. They exhibit little contribution to absorption enhancement while dramatically increase the difficulty in the device fabrication.

However, these pitfalls in using high-permittivity scattering material are overcome by the proposed GA based NGTO with the discontinuous Heaviside density filter. In this test, a 64×64 mesh with filtering radius r = 3 is applied. The optimized scattering patterns consisting 3x3 unit cells for incident wavelength of 400nm, 500nm and 600nm are shown in Figs.2 (g), (h) and (i), respectively. Compared with the case using low-permittivity scattering material, the more complicated physics leads to more complex geometries in the optimized designs to provide effective scattering. The absorption coefficients of the optimized performances at each wavelength are summarized in the third row of Table. 1. All optimized designs achieve near-complete absorptions, ranging from 0.96 to 0.99, at the targeting wavelength without using the back reflector. These results prove that both reflection and transmission are eliminated and the whole diffracted energy is absorbed by the active layer through optimization. In the spectral performance plots shown in Figs.2 (j), (k) and (l), the distinctive absorption peaks at each target wavelength illustrate the effectiveness of optimization, whereas the numerous sharp peaks over the spectrum reveal the severe physical resonances for this design concept.

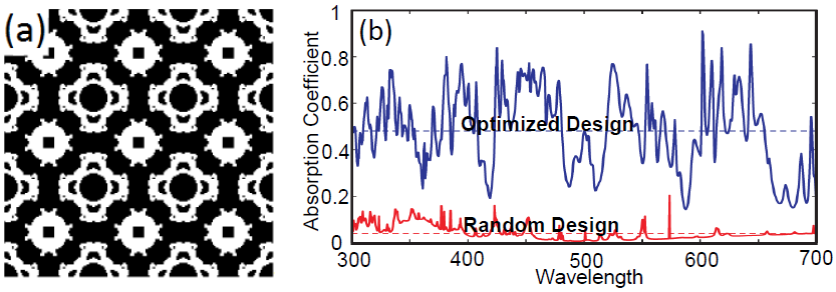

Figure 3: Broadband optimized design using GA based NGTO with high-permittivity scattering material

Finally, an optimization of light trapping structure over the broad visible spectrum from 300nm to 700nm is performed. Designing proper scattering patterns for broadband performance becomes even more complicated than for a single wavelength. As slot waveguide supports discrete resonances, the spectral absorption depends on contributions from the aggregated resonances. It is expected that the overall spectral absorption can be enhanced with the improvement of absorption of multiple wavelengths. Therefore, 31 wavelengths evenly distributed in the spectrum are considered in this broadband optimization. The optimized pattern and the spectral absorption from 300nm to 700nm are shown in Figs.3 (a) and (b) respectively. The average absorption over the whole spectrum reaches 0.481, with a light-trapping enhancement factor[39] of 24.4, which is above three times the Yablonovitch Limit at the normal incidence. For comparison, the spectral absorption of the random scattering layer using the same material is depicted in Fig.3 (b). In contrast to both the strong coupling to slot waveguide modes and reduction of reflection from optimized scattering patterns, the random scattering pattern provides a continuum of wave vectors and results into a much lower absorption coefficient of 0.04 and an enhancement factor 2.03 that is inferior to the Yablonovitch Limit. This demonstrates that without elaborate designs of the topology of scattering

layer, slot-waveguide based cells cannot exhibit superior spectral performance.

6. SIMP based GTO versus GA based NGTO for Light-trapping Structure Optimization

6.1. SIMP based GTO Approach

While the proposed GA based NGTO approach has been successfully applied to achieve highly efficient light-trapping structures, the SIMP based GTO approach is also implemented in this study for the purpose of comparison. The SIMP method [35] is presently the most popular GTO method. The original discrete value (0-1) problem is relaxed to a continuous variable optimization problem to enable the gradient calculation. The intermediate pseudo density value between 0 and 1 is penalized with a power law. Using appropriate filtering techniques [43], an almost 0-1 discrete design can be obtained as the optimization results for certain problems.

Recent years have seen successful applications of the SIMP method in designing high-performance nanophotonic devices [28, 40, 56]. In typical nanophotonic optimization problems [57], such as the low-loss waveguide design, the discrete 0-1 structure with sharp material contrast on the boundary is favored. For this reason, P is chosen to be 1 in the SIMP interpolation scheme for permittivity. Nevertheless for the nanophotonic light-trapping structure design, our study shows that optimization may converge to designs with large amount of intermediate-valued elements even with a penalization factor P = 3. Such design is infeasible for the photolithography based fabrication. The density filtering with an approximated Heaviside function [43, 58] was claimed to be effective in achieving 0-1 discrete results. Instead of the non-differentiable true Heaviside step function, a continuous approximation is adopted in this filter [43]. A pure 0-1 discrete design is achieved by gradually increasing the curvature parameter β in the approximated Heaviside function using a continuation method. While this filter is effective for mechanical structure optimizations, limited application to nanophotonic designs is found in literature. According to our tests, the β continuation not only increases significantly the number of iterations to convergence, but also causes perturbation to optimization at each continuation step. More importantly, a large magnitude of β adds additional nonlinearity to the nanophotonic light-trapping structure design; optimization may be trapped at a design of poor performance.

In this work, we use the modified Heaviside density filter [59], which is termed as the constant Heaviside density filter in this paper. The β continuation is eliminated by increasing the upper bound of the design variables x_i from 1 to x_{max}. The issue of intermediate-valued density can be effectively suppressed by ensuring a large magnitude of $\beta \cdot x_{max}$.

For the forward analysis model, the RCWA (see Section 4.3), the same analysis model used in the GA based NGTO is adopted for the SIMP based GTO. The gradient information is obtained by calculating the sensitivity of the absorption coefficient to the material property, i.e. the permittivity $\boldsymbol{\varepsilon}$, based on the RCWA. The method proposed in [60] to compute the gradient information based on the RCWA for 1D grating structure parametric design is extended in this work for 2-D topology optimization of light-trapping structure. This analytical gradients computation involves calculating the eigenvalues and eigenvectors sensitivities of the field governing eigen-equation for the scattering layer and efficient matrix manipulation for S matrix algorithm. It should be noted that the finite-difference gradient information becomes singular at certain positions for this problem. This singularity exposes a strong nonlinearity due to the physical resonance.

With the gradient information, a design is updated using the method of Moving Asymptotes (MMA) optimizer [61]. As recommended in [59, 61], a conservative MMA with tightened asymptotes (compared with the default settings provided in [62]) is adopted to prevent oscillations in optimization process considering the high nonlinearity of this problem. For a comprehensive comparison, both the low and high-permittivity scattering material cases are tested and compared to the results using GA based NGTO.

6.2 Comparison between SIMP based GTO and GA based NGTO

Considering the distinct physics governing the slot-waveguide based thin-film solar cell using different scattering materials as shown in Section 5, a comparison between the SIMP based approach and the GA based approach is conducted based on the cell model shown in Fig.1 (c). It has been discovered so far that using low-permittivity scattering material results into a less nonlinear design problem with limited physical resonance, whereas the high-permittivity material in the scattering layer leads to a highly nonlinear problem with severe resonance. The performance of the two topology optimization algorithms in handling these two categories of behaviors will provide insights into the applicability of the two algorithms under different conditions.

Comparison 1: Slot Waveguide based Solar Cell with Low-permittivity Scattering Material

In this comparison, the solar cell structure is shown in Fig.1 (c) with a low-permittivity scattering material. The unit cell is discretized using a 64×64 mesh without any symmetry constraint on geometry. Two incident polarization angles of $\pi/4$ and $3\pi/4$ are simultaneously applied for proving the advantage of symmetric geometry in designing periodic light-trapping structures. The constant Heaviside density filter without β continuation is adopted with $r = 3$, $\beta = 2$, and $x_{max} = 3$, where r denotes the filtering radius. The penalty factor P in SIMP scheme

is set as 3 to mathematically suppress the intermediate-valued density.

The optimized designs (3×3 cells array) for incident wavelength of 400nm, 500nm and 600nm using SIMP based GTO starting from random designs is shown in Figs.4 (a), (b) and (c), respectively. By comparing with Figs.2 (a), (b) and (c), it is observed that the GTOs converge to the very similar designs as those from NGTO. This significant similarity verifies the validity of using both approaches in delivering efficient nanophotonic light-trapping structure. Moreover, since no symmetry constraint is imposed in this test, the appearance of the symmetric geometry in optimized designs proves the superiority of symmetric geometry in periodic structure for light trapping under the natural condition of complete incident polarizations. Figs.4 (d), (e) and (f) show the optimization histories of the absorption coefficient value and the maximum magnitude of design change. Owning to the simplified physics in the cell with low-permittivity scattering material, no significant oscillation appears at the latter stage of the optimization. Convergence is achieved within 100 iterations for all optimizations at different wavelengths. The absorption coefficients of the optimized designs using the SIMP based approach are summarized in the second row of Table 4. It shows that the SIMP based GTO achieves close, albeit lower values of absorption coefficient in the optimized designs comparing to those from NGTO shown in Table 1. As discussed in 3.2, the simplified physics in this case results into a solution space with less local optimum. Moreover, the mild scattering effect provided by the low-permittivity scattering material leads to limited resonance. As the result, the SIMP approach and the GA approach achieve similar designs for this comparison.

It is noted from comparing the results in Table 1 and Table 2 that the optimal performance from using SIMP is slightly inferior to the GA optimized results. This is attributed to the intermediate-valued elements on the boundary of the structure from using the SIMP method. The performances of most nanophotonic devices are sensitive to small structural perturbation. For instance, the optimization for 400nm incidence leads to a design with a large amount of intermediate-valued elements (Fig.4 (a)) and a topology slightly different from that of NGTO shown in Fig.2 (a). This issue may be mitigated by using a larger product of $\beta \cdot x_{max}$ in the constant Heaviside density filter. Nevertheless, even for the optimized designs of 500nm and 600nm incident wavelengths, where intermediate-valued elements are effectively suppressed, a post process is necessary for pure 0-1 designs required by the photolithography fabrication. Yet, a simple post process is risky considering the structural perturbation sensitiveness of nanophotonic devices.

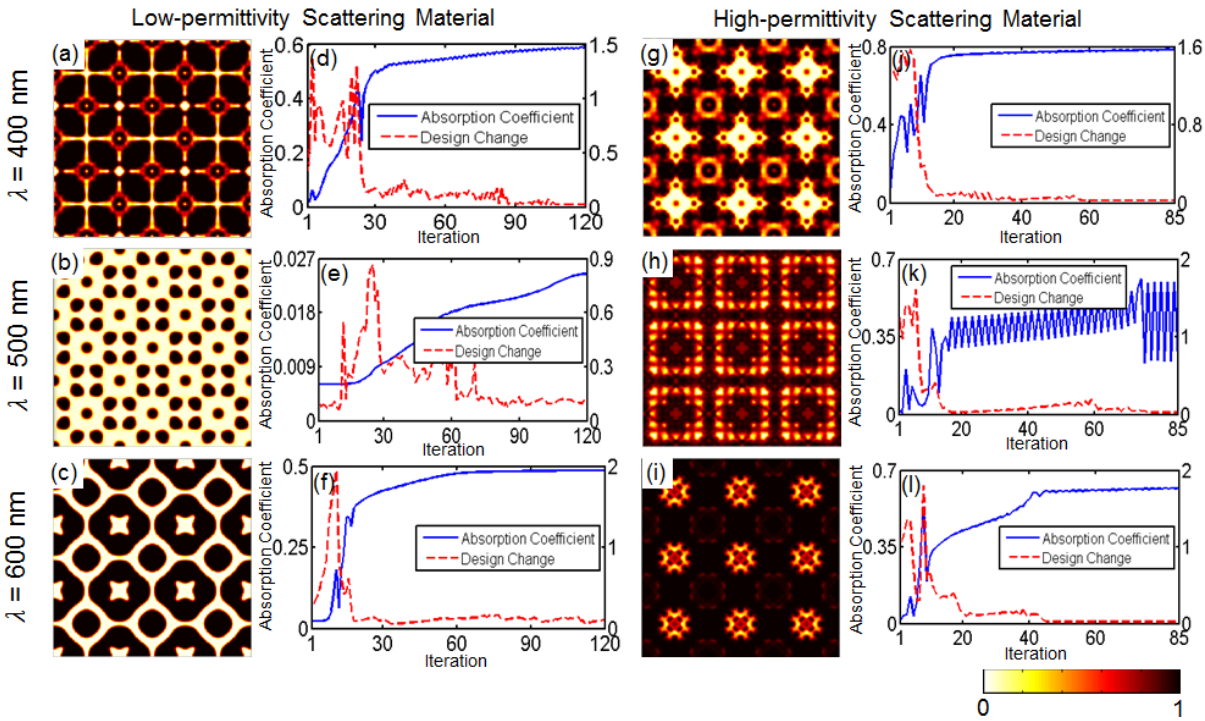

Figure 4: Optimized results using SIMP based GTO

Table 2: Absorption Coefficient of Optimized Design using SIMP based GTO

Targeting Wavelength	λ = 400 nm	λ = 500 nm	λ = 600 nm
Low-permittivity Scattering Material	0.611	0.026	0.488
High-permittivity Scattering Material	0.805	0.601	0.622

Comparison 2: Slot Waveguide based Solar Cell with High-permittivity Scattering Material
In this comparison, the high-permittivity material is used in the scattering layer of the slot waveguide based cell. While there is a potential to achieve a complete absorption as shown in Fig.1 and Table 1, the strong scattering effect and the complex physics with competing governing processes result in a large number of local optimum in the solution space and severe resonance for the problem, posing a great challenge to gradient based approaches. With the same optimization condition as that in the previous comparison, the results using SIMP approach for this high-permittivity scattering material case at 400nm, 500nm and 600nm incident wavelengths are shown in Figs.4 (g), (h) and (i). The corresponding absorption coefficients are displayed in the third row of Table 2. Compared with the results shown in Fig.1 and Table 1 using GA based approach, it is noted that the SIMP approach fails in achieving high-performance designs for this complicated case using high-permittivity scattering material. The SIMP approach mainly suffers from the intermediate-valued elements, the strong physical resonance and the local optimum issue. For examples, a blurred design shown in Figs.4 (g) is obtained with a large number of intermediate-value elements for the 400nm incidence case; the resonance leads to the strong oscillation in the 500nm-incidence optimization process as shown in Fig.4 (k); and the 600nm-incidence optimization converges prematurely to a poor-performance local optimum as shown in Figs.4 (i) and (l). Efforts have been made in this research to improve the regularization scheme of the SIMP based approach, as discussed next.

6.3. Extension on SIMP based GTO Approach
In this section, two regularization techniques are tested aiming for overcoming the aforementioned difficulties experienced by the SIMP approach. First, the constant Heaviside density filter with a larger $\beta \cdot x_{max}$ is adopted to suppress the intermediate-valued elements in the 400nm-incidence optimization cases with both the low-permittivity and high-permittivity scattering materials as shown in Figs.4 (a) and (g), respectively. Next, a continuation scheme aiming for suppressing the resonance issue in the high-permittivity scattering case is applied to optimization at 500nm and 600nm incidences.

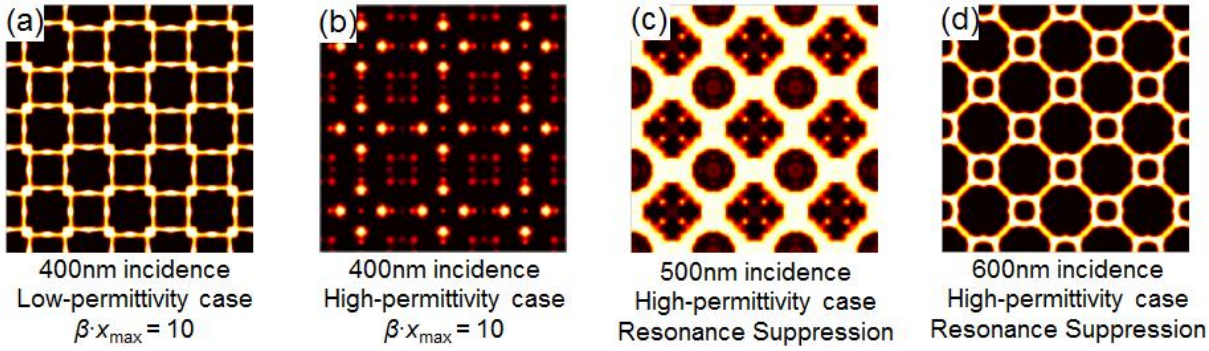

Figure 5: SIMP based NGTO with large $\beta \cdot x_{max}$ in Heaviside density filter or with resonance suppression scheme

To further suppress intermediate-valued densities, a constant Heaviside density filtering with a larger $\beta \cdot x_{max}$ is applied. We increase the design variable upper-bound x_{max} from 3 to 5 with β fixed at 2 as recommended in [59]. Figs. 5 (a) and (b) show the optimized results (3×3 cells array) for the incident wavelength of 400nm using the low-permittivity and the high-permittivity scattering materials, respectively. For the low-permittivity scattering material case shown in Fig. 5(a), the intermediate-valued elements are effectively suppressed. Hence, a more discrete design is obtained with an improved absorption coefficient of 0.701 and a similar topology as that from using GA based approach shown in Fig.2 (a). On the contrary, the increased magnitude of $\beta \cdot x_{max}$ results into an inferior design (Fig. 5 (b)) for the high-permittivity scattering material case with high nonlinearity. The absorption coefficient of the optimized design is reduced to 0.728. In this case, we found that the optimizer's ability in adjusting material distribution is restrained and the optimization converges prematurely to a design of inferior performance. In contrast, the GA based NGTO approach presented earlier is capable of delivering highly efficient structures with pure 0-1 designs and near-complete absorption in facing the challenges of using high-permittivity scattering material.

To suppress the resonance issue in the high-permittivity scattering which results in local optimums in, a scheme of adding artificial damping with a continuation method proposed in [56] is extended in this research. Here we apply a continuation scheme to artificially restrain the absorbing ability of the active layer at the early stage of the optimization for resonance suppression. Specifically, we start the optimization with the magnitude of the image part in the active material permittivity as 20% of the true magnitude, and increase the fraction until it reaches 100% of the true magnitude at the end of the optimization. In this case, the strong resonances over the numerous local optimums are expected to be suppressed at the beginning, and the optimization is expected to converge toward a

promising direction. This scheme is applied to the optimizations for the high-permittivity scattering material case targeting at 500nm and 600nm incident wavelengths. For the constant Heaviside density filter, β and x_{max} are fixed at 2 and 3 respectively. The optimization results are shown in Figs.5 (c) and (d) for incident wavelength of 500nm and 600nm respectively. By using the resonance suppression scheme, the 500nm-incidence optimized design in Fig.5 (c) achieves an absorption coefficient of 0.825 and the 600nm-incidence optimized design in Fig.5 (d) achieves an absorption coefficient of 0.910. Comparing with the corresponding results in Table 2 without the resonance suppression scheme, it is discovered that designs with better performance are achieved by applying this scheme. In spite of the efforts, the near-complete absorptions are not achieved and the 500nm-incidence case shown in Fig.5 (c) still suffers from intermediate-valued elements.

7 Conclusion

This paper presents a general, yet systematic design approach based on topology optimization for designing highly efficient nanophotonic light-trapping structure in solar cell beyond the reach of conventional intuitive designs. By exploiting the power of topology optimization, this approach searches for the optimal topology with simultaneous consideration of all governing physics over the optical absorption and the robustness of algorithm in dealing with strong nonlinearity involved in the nanophotonic light trapping. Through a comprehensive comparison between the GA based NGTO approach and the SIMP based GTO approach to the same application, insights into both approaches in dealing with nanophotonic design problems is obtained.

For the proposed GA based NGTO approach, the introduction of the discontinuous Heaviside density filter effectively prevents the numerical instability involved in the GA and topology optimization. In demonstrating this approach, solar cell models with the corresponding light-trapping process governed by differing physics are tested, including the slot-waveguide based cell with low-permittivity scattering material and high-permittivity scattering material. The use of low-permittivity scattering material simplifies the physics in slot-waveguide based nanophotonic light-trapping process and reduces the nonlinearity of the design problem. The high-permittivity material in the scattering layer of the slot-waveguide based cell leads to a highly nonlinear problem, which poses a challenge to the design approach. In spite of the distinct physical characteristics, highly efficient light-trapping structures are obtained for these cases using the GA based NGTO approach. The optimized designs are shown to achieve significant enhancements in light absorption and exceeding the Yablonovitch limit in light-trapping effect. We have fabricated the design of the scattering layer shown in Fig.3 (a) using the electron beam lithography. This optimized organic solar cell design requires much less materials, hence lower manufacturing cost, while still maintaining the efficiency. Therefore, there is a great potential of using the solar cell as a cost effective alternative energy source.

In comparing the GA based and the SIMP based approach for light-trapping structure design, both the low-permittivity and the high-permittivity scattering material cases for slot-waveguide based solar cell are tested. For the low-permittivity scattering material case with mild physical resonance, these two approaches converge to the similar designs. As a comparison, GA based approach achieves pure 0-1 design with superior absorbing performance that is ready for fabrication. The SIMP based approach is more efficient in delivering the optimization results. Based on our exploration for this light-trapping structure design problem with a limited number of design variables, the SIMP based approach is at least 5 times faster than the GA based approach to convergence under the same computing environment. This efficiency can be further improved by utilizing the adjoint approach in gradient evaluation, which is not included in this comparative study. However, the optimized designs from SIMP based approach suffer from the issue of intermediate-valued density which results into lower absorption. This issue can be mitigated, yet not eliminated by appropriate filtering techniques with careful parameter tuning in the less nonlinear problem. For the more challenging case with high nonlinearity, the GA based approach significantly outperforms the SIMP based approach in generating highly efficient design with fabrication feasibility. In contrast, the SIMP based approach not only encounters the intermediate-valued desnity issue, but also faces the challenge of local optimums and optimization oscillations due to the severe physical resonance involved. The effort in tuning the filter is shown to be ineffective in this case. Therefore, a continuation scheme aiming at suppressing resonance during optimization is proposed and tested. With this scheme, the chance of being trapped at local optimum with poor performance is reduced and improved optimization results may be obtained. However, the improved designs are still inferior compared with the results using GA based approach. Based on the comparing study, the GA based NGTO approach is recommended for certain nanophotonic designs where the number of design variable is limited and strong nonlinearity is involved, such as the case of slot-waveguide based solar cell using high-permittivity scattering material. Nevertheless for the nanophotonic optimization problems without strong resonance, such as the low-permittivity scattering material case, and the problems involving large number of design variables, the SIMP based approach and other GTO methods are recommended if the issue of intermediate-valued density is well resolved.

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