Discrepancy-Based Genetic Algorithm Optimization of Quasi-Random Nanostructures for Broadband Light Reflection Mitigation

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Abstract— **Periodic nanostructures have previously been used to increase the absorption of various semiconductors, but they mainly provide improvement in a specific spectrum. On the other hand, random nanostructures can increase the adsorption over a broad range of frequencies without a targeted frequency. Instead, quasi-random nanostructures have shown broad spectrum improvements and targeted spectrum enhancement compared to both periodic and random nanostructures. Considering an infinite number of quasi-random nanostructures, it is challenging to design or optimize a quasi-random structure pattern via traditional simulations (i.e., Finite Difference Time Domain (FDTD), Finite Element Analysis, Rigorous coupled-wave analysis). Discrepancy is a method of measuring surface randomness of a structure. Previous work has shown that a higher star discrepancy, and there for a higher surface randomness, of a quasi-random structure reduces surface reflection and increases optical path length, resulting in a higher absorption for semiconductors. Therefore, discrepancy calculations allow a quasi-random nanostructure to be evaluated more efficiently than running a FDTD simulation. In this paper, we used a genetic algorithm (GA) to optimize the discrepancy of quasi-random nanostructures instead of running thousands of optical simulations for the optimization. The optimized quasi-random sequence is compared with a classical quasi-random Fibonacci sequence. The star discrepancy, or the maximum absolute discrepancy was measured and found to be 0.0026 for a Fibonacci sequence and 0.0387 for the GA generated sequence, an order of magnitude enhancement. The FDTD simulations show that the GA-based quasi-random nanostructure shows a 20% absorption improvement over the Fibonacci sequence at 450 nm wavelength and additionally shows a doubling of absorption in the near-infrared region, suggesting a better antireflection performance.**

Keywords— Quasi-random, nanostructures, anti-reflective coating, Genetic Algorithm

I. Introduction

Structured anti-reflective coatings have long since provided a way for researchers to reduce reflection losses at the interfaces between layers. The main mechanisms that reduce the reflections are more multiple reflections between the structures and a gradual reduction of the refractive index between layers. The structures that have seen the most prominent adoption have been periodic structures, such as the Moth eye structure [1], nano-cubes, nano-hexagons, nano-rods, etc. [2] which have been shown to provide great anti-reflective properties for a specific wavelength. Random nanostructures, on the other hand, typically provide a lower specific wavelength improvement compared to periodic structures but show greater improvement over the broadband spectrum.

Quasi-random structures combine the broadband improvements of the random structures with the higher performances of periodic structures. A quasi-random structure is a structure that appears random locally but remains ordered at larger length scales. Previous studies have shown that discrepancy provides a way to quantitatively compare quasi-random structures for anti-reflective properties [3].

2D discrepancy calculation quantifies how well a matrix is equidistributed. A lower discrepancy sequence is more equally distributed. Where *P* is a set of numbers, *A(B;P)* is the number of points *P* that are in *B*, *J* is the set of boxes, *B* is the sub area being evaluated, and *N* is the number of points in J. λ_s is the s-dimensional Lebesgue measure. For a 2D sequence, the Lebesgue measure is equivalent to the ratio between the area of B and the area of J.

$$D_N(P) = \sup_{B \in J} \left| \frac{A(B;P)}{N} - \lambda_s(B) \right| \tag{1}$$

In terms of this experiment, *J* is the matrix representing the pattern being optimized. The matrix is filled with ones or zeros to represent pits and lands respectively. B is then the subarea being evaluated.

$$D_N(P) = \sup_{B \in J} \left| \frac{Number\ of\ 1s\ in\ B}{Number\ of\ 1s\ in\ J} - \frac{Number\ of\ entries\ in\ B}{Number\ of\ entries\ in\ J} \right| \tag{2}$$

Then star discrepancy, D*, is the maximum discrepancy of all subareas, B. A quasi-random pattern can then be constructed using the inequality [3].

$$D_N^*(x_1, \dots, x_N) \le C \frac{(\ln N)^s}{N} \tag{3}$$

Genetic Algorithms (GA) are a category of algorithms that are inspired by the natural process of selection. They have been

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widely used in many fields, from solar cell research [4] to medicine [5]. In this paper, an initial population of data points are generated and then evaluated. The best performing data points are selected as the parents for the next generation of data points. That next generation has traits from the parents, but also have some random features due to mutations. Genetic algorithms previously used in the solar cell field have relied on time intensive FDTD evaluations to select the best patterns. By changing the evaluation function from reflectance, determined by a FDTD simulation, to star discrepancy, a matrix can be evaluated in seconds rather than hours. Then, once the GA has converged to a solution, a singular FDTD simulation can be run to determine its optical properties.

II. RESULTS AND DISCUSSION

A quasi-random pattern was generated using the genetic algorithm from MATLAB. Discrepancy was used as the objective function. This pattern was then drawn with 0s corresponding to pits and 1s corresponding to lands. A known quasi-random sequence, the Fibonacci sequence, was used as a comparison point. The 2D filling ratio was 0.478 for the GA sequence and 0.6176 for the Fibonacci sequence.

Figure 1: Fibonacci sequence on the left and GA pattern on the right

Figure 2 shows the schematic of the solar cell simulated. Each layer has a 1 µm thickness: silicon (red), PDMS (blue), PDMS Structure (blue). Each edge is 11 µm long.

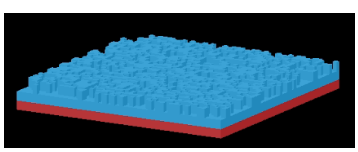

Figure 2: Solar Cell Schematic

Each pit/land was 220 nm wide, 220 nm long, and 1 µm thick. The FDTD simulation was run with a minimum mesh size of 50 nm and an accuracy of 7.

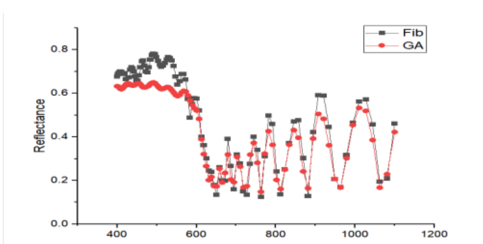

Figure 3: Reflectance vs Wavelength for the two patterns

Fig.2 shows the reflectance as a function of wavelength for both GA optimized nanostructured coating and Fibonacci coating. Fig. 2 shows that the reflectance of the GA pattern is 20% lower than the Fibonacci sequence in the 400nm to 550nm range. There were also reductions of the peak reflectance in the rest of the spectrum. These reductions of reflection are in part due to the filling ratio of the GA pattern being closer to 0.5, as a more even split of pits to lands would cause a more gradual change of index of refraction between the air and the base PDMS coating. Additionally, the GA pattern promotes greater internal reflection between the nanostructures, as the surface is more random.

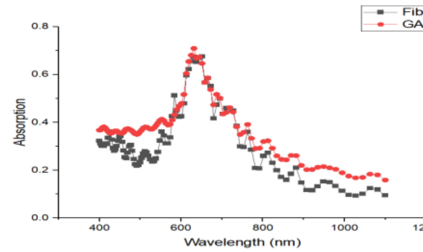

Figure 4: Absorption vs Wavelength for the two patterns

Fig. 3 depicts the absorption as a function of wavelength for GA optimized coating and Fibonacci coating. Fig. 3 shows that the absorption of the system improved throughout the entire wavelength spectrum tested. Notably, the absorption of the system doubled from 0.2 to near 0.4 at 500 nm and again doubled at 1000 nm from 0.1 to 0.2. The improvements before 600 nm are from the reflection reductions, as the absorption is the complement to reflectance; however, the improvements past the 800 nm range are from a combination of reflectance and transmission reduction. As little improvement is seen in the reflectance of the system at 1000 nm, but there is still an absorption increase, the optimized pattern also directly improved the absorption of the system through light trapping.

III. CONCLUSION

A genetic algorithm was used to generate and optimize a quasi-random sequence to reduce reflectance of a silicon solar cell. Discrepancy was used as the objective function. The GA optimized pattern showed a 20% improvement in reflectance over the Fibonacci sequence at 500nm and a doubling of absorption at 1000 nm. These results are partially due to a change in filling ratio, but also due to increased light trapping.

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