Optimal Design of Graded Refractive Index Profile for Broadband Omnidirectional Antireflection Coatings Using Genetic Programming

Yongxiang Zhao\textsuperscript{1, 2, *}, Fei Chen\textsuperscript{2, 3}, Qiang Shen\textsuperscript{2}, and Lianmeng Zhang\textsuperscript{2}

Abstract—To eliminate the average reflectance of antireflection coatings to the greatest extent, a Genetic Programming (GP) algorithm is proposed to design and optimize the graded refractive index distribution profile for broadband omnidirectional antireflection coatings. The proposed GP-index profile in this paper can obtain an extremely low average reflectance of $4.61 \times 10^{-7}\%$ over a wide range of incident angles and wavelengths which is obviously superior to the average reflectance of $8.09 \times 10^{-3}\%$, $3.29 \times 10^{-4}\%$ and $4.35 \times 10^{-5}\%$ for linear profile, cubic profile and quintic profile. That means, Fresnel reflection almost can be eliminated by the optimal GP-index profile for omnidirectional incidence over a broad wavelength range. Moreover, it is demonstrated the proposed GP-index profile has better robustness, and it still has the best broadband and omnidirectional antireflection characteristics for the TiO$_2$/SiO$_2$ graded-index AR coating. Therefore, the proposed GP-index profile is obviously superior to the conventional linear profile, cubic profile and quintic profile, and the design methodology presented in this paper that uses a genetic programming technique is a quite convenient means to pursue an optimal nonlinear refractive index profile with broadband and omnidirectional antireflection characteristics.

1. INTRODUCTION

Minimizing optical reflection at dielectric interfaces has long been a fundamental yet vital subject in various applications in optics. The most well-known antireflection (AR) coating may be the quarter-wavelength coating having a refractive index equal to the geometric mean of the indices of two different materials. However, performance of such quarter-wavelength coating falls off when deviating from normal incidence or the designed wavelength, and omnidirectional and broadband antireflection characteristics are often required for applications such as solar cells or image sensors. For example, depending on the materials used for the absorbing layers, the typical spectral range of modern solar cells is in general from 350 nm to 1200 nm. Furthermore, in the absence of the sunlight tracking system, lower angle-averaged reflectance at the top surface of solar cells over a wide angle of incidence up to 80° or larger will be also essential to guarantee a higher collection efficiency throughout the day. Therefore, an AR coating with broadband and omnidirectional antireflection characteristics is highly desirable and may still remain a challenge for solar cell devices.

The pursuit of low-reflectivity coatings has fascinated researchers for more than a century. In 1880, Lord Rayleigh analyzed reflections of waves from graded interfaces between two dissimilar media, and realized that “the transition may be so gradual that no sensible reflection would ensue” [1]. That means, for an infinitely thick, continuously graded AR coating, Fresnel reflectivity approaches zero. Recently, several continuous design methodologies and implementation by using nanoporous materials have been published on high-performance broadband graded refractive index AR coatings [2–5].
Significant research has focused on finding graded refractive index profiles which minimize reflection for a given AR coating thickness. A linear profile is a reasonable starting point, but other profiles, such as the cubic profile and quintic profile, have been found to give superior performance [2, 6].

The governing equations of three general profiles including linear profile, cubic profile and quintic profile are given by

\[ n = n_{low} + (n_{high} - n_{low}) x \]
\[ n = n_{low} + (n_{high} - n_{low}) (3x^2 - 2x^3) \]
\[ n = n_{low} + (n_{high} - n_{low}) (10x^3 - 15x^4 + 6x^5) \]

where \(n_{low}\) and \(n_{high}\) are the refractive indices of the incident and substrate media, respectively, and \(x\) is the relative thickness of AR coatings whose range is \(0 \leq x \leq 1\). It has been reported that the quintic-index profile is near the optimum profile for a graded-index antireflection coating [2, 7].

However, given the capability of producing continuously varying refractive-index coatings, what is the optimal index distribution, linear profile, cubic profile, quintic profile or any other profile?

In order to answer the above-mentioned question, a systematic study on design of graded refractive index profile for broadband omnidirectional antireflection coatings is performed in this paper. Firstly, Genetic Programming (GP) algorithm is proposed to design and optimize the graded refractive index profile for broadband omnidirectional antireflection coatings. The proposed GP-index profile can obtain an extremely low average reflectance of \(4.61 \times 10^{-7}\%\) over a wide range of incident angles and wavelengths in comparison with linear, cubic and quintic profiles. Moreover, to further verify the robustness and universality of the optimal GP-index profile proposed in this paper, we have compared the broadband and omnidirectional antireflection characteristics of linear profile, cubic profile, quintic profile and optimal GP profile for another TiO\(_2\)/SiO\(_2\) graded-index AR coating. It is demonstrated the proposed GP-index profile has better robustness, and it still has the best broadband and omnidirectional antireflection characteristics for the TiO\(_2\)/SiO\(_2\) graded-index AR coating.

2. GP-BASED DESIGN AND OPTIMIZATION MODEL

There exist many limitations in order to achieve optimum antireflection characteristics from linear profile, cubic profile or quintic profile. (i) Such profiles are all fixed designs, where there is no room for considering important parameters, such as refractive-index dispersion of coating and substrate materials, and spectral distribution of incident light, etc. for application-specific optimization. (ii) Such profiles are obtained by changing the governing equations based on human intuition, experience or large numbers of simulation experiments which were time-consuming, ineffective or expensive. Therefore, an effective and systematic methodology for guiding and designing the optimal graded refractive index profile with broadband and omnidirectional antireflection characteristics is quite desirable and vital.

Heuristic search techniques have been successfully applied to many electromagnetic problems to pursue novel solutions which are difficult to obtain using the conventional design approaches. For instance, genetic algorithms (GAs) have been used to optimize wide frequency band of negative index metamaterials [8], scannable circular antenna arrays [9], and fractal antenna-array [10]. Differential evolution (DE) algorithm has also been used to optimize low loss negative index metamaterials [11, 12], graded SiNx and SiOxNy antireflection coatings [13], graphene transparent electrodes [14], and so on.

Genetic programming (GP) is a new heuristic search approach which is an extension of the conventional genetic algorithm (GA), generating novel solutions to complex problems, developed by Koza [15]. Unlike the cubic and quintic profiles, the genetic programming is an optimization design method with which any figure of merit can be taken into consideration. Using the concepts borrowed from biology, namely, selection, recombination and mutation, optimal graded refractive index profile can be obtained.

Moreover, the genetic programming is a practical and application-specific optimization method because factors, including angles of incidence and relative weighting of the solar spectrum, can both be considered to achieve a global optimum performance in a specific condition.

Therefore, in this paper, genetic programming algorithm is employed to design and optimize the graded refractive index profile for broadband omnidirectional antireflection coatings in order to decrease the average reflectance of AR coatings to the greatest extent.
This paper will address the question of AR coating design with graded-index media. That is, given the capability of producing continuously varying refractive index coatings, what is the optimal refractive index distribution profile to minimize the average reflectance of AR coatings for a wide range of incident angles and wavelengths?

For simplicity, we have restricted ourselves in this paper to the problem of making glass interfaces antireflecting over the visible wavelength from 400 nm to 700 nm. Figure 1 depicts the schematic of a 1000 nm graded-index AR coating between incident media and substrate media with \( n_i = 1.6 \) and \( n_s = 2.4 \) which refer to the literature [2].

![Figure 1. Schematic of a 1000 nm graded-index AR coating between incident media and substrate media with \( n_i = 1.6 \) and \( n_s = 2.4 \).](image)

The block diagram of the GP design for parameters optimization has been illustrated in detail in the literature [15]. In GP, the individual solutions of a problem are represented as program trees composed of nodes and arcs. Nodes without outgoing arcs are terminals. Nodes with one or more outgoing arcs are functions that act on terminals or other functions. The terminal and function sets are important components of a genetic program since they make up the structure of the genetic program. The terminal set for the refractive index distribution profile consists of variable \( x \) and constants, where variable \( x \) is the relative thickness of AR coatings and the constants are floating point numbers. In this paper, the random floating point numbers within the range \([-10, 10]\) are added to the set of terminals to increase the genetic diversities of the refractive index distribution profile. The function set consists of various mathematical functions, such as addition, subtraction, multiplication, division, and potentially other more complex functions. The size, shape, and structure of the solution as a genetic program are left unspecified and are found by using the genetic programming operators (i.e., selection, recombination and mutation). Solving a problem therefore becomes a search through all possible combinations of symbolic expressions defined by the programmer.

Moreover, in the traditional GP evolution process, the candidate parents are always chosen stochastically for mutations or crossover which could not guarantee that the population will become more and more successful with the passing of generations. However, in our work, an “Elite strategy” is employed in GP evolution process. That means, the best individual is “cloned” or retained from each generation to the next. Crossover and mutation are not applied to these elite individuals, i.e., they are simply copied. This guarantees that if the fitness function remains the same, the success of a generation will be, at least, no worse than that of the preceding generation.

In this paper, the goal of GP is to pursue the optimal refractive index distribution profile to minimize the average reflectance of AR coatings for the wavelength range of 400–700 nm and angles \( 0^\circ–90^\circ \). Therefore, the fitness function of GP can be defined as follows:

\[
\text{Minimize: } R_{\text{ave}}(\lambda, \theta) = \frac{1}{\lambda_2 - \lambda_1} \frac{1}{\theta_2 - \theta_1} \int_{\lambda_1}^{\lambda_2} \int_{\theta_1}^{\theta_2} \left( \frac{R_{\text{TE}}(\lambda, \theta) + R_{\text{TM}}(\lambda, \theta)}{2} \right) d\theta d\lambda
\]

In the Eq. (4), \( \lambda_1 \) and \( \lambda_2 \) are equal to 400 nm and 700 nm, respectively. And \( \theta_1 \) and \( \theta_2 \) are equal to 0 and \( \pi/2 \), respectively. Moreover, \( R_{\text{TE}} \) and \( R_{\text{TM}} \) are the angle and the wavelength-dependent reflection coefficients for \( TE \)- and \( TM \)-polarized light modes, respectively.
3. DESIGN RESULTS AND DISCUSSION

The parameters for the GP optimization are listed in Table 1. When we calculate the reflection coefficients of AR coatings, a fixed thickness coating is divided into 1,000 sublayers of equal thickness. The reflectivity at several wavelengths over the spectrum is evaluated by using transmission-line theory [16–20].

The convergence curves of GP for the refractive index distribution profile optimization are presented in Figure 2. From Figure 2 it can be seen that the GP algorithm almost converges before the maximum number of the generation is reached.

The optimal GP-index profile at 10, 100, 500 and 1000 generations are listed in Table 2. In the optimal GP-index profile results presented in Table 2, there are three floating point numbers in $F(x)$ which are $-0.8749$, $-1.5777$ and $-2.1941$ respectively. These floating point numbers within the range $[-10, 10]$ are generated randomly, and are added to the terminal set of GP to increase the genetic diversities of the refractive index distribution profile. From the optimization results of Table 2, it can be seen that the objective function $R_{\text{ave}}(\lambda, \theta)$ of GP is getting smaller and smaller which decreases from

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
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<tbody>
<tr>
<td>Population Size</td>
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<tr>
<td>Recombination Probability</td>
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<td>Mutation Probability</td>
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<td>Selection Strategy</td>
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<td>Maximum Generations</td>
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<td>Maximum Tree Depth for Initialization</td>
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<tr>
<td>Maximum Tree Depth for Recombination and Mutation</td>
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<tr>
<td>Initial Population Creation Method</td>
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<tr>
<td>Terminal Set</td>
<td>${+, -, \times, /}$</td>
</tr>
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</table>

Table 1. Parameters for the GP optimization.

<table>
<thead>
<tr>
<th>Generation</th>
<th>$R_{\text{ave}}(\lambda, \theta)$ (%)</th>
<th>Optimal GP-index profile $n = n_{\text{low}} + (n_{\text{high}} - n_{\text{low}})F(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$4.29 \times 10^{-3}$</td>
<td>$F(x) = (x - 1.5777 \times (x * x) * x) * x * x$</td>
</tr>
<tr>
<td>100</td>
<td>$2.14 \times 10^{-4}$</td>
<td>$F(x) = (x + (((x * x - x) * (-1.5777)) * (((x + (((x * x) * x - x - 0.8749) \times x) + (((x * x) * x - x) * x) * x) * x) * x) * x) * x)$</td>
</tr>
<tr>
<td>500</td>
<td>$1.29 \times 10^{-6}$</td>
<td>$F(x) = (x + (((x * x - x) * (-1.5777)) * (((x + (((x * x) * x - x - 0.8749) \times x) + (((x * x) * x - x) * x) * x) * x) * x) * x) * x)$</td>
</tr>
<tr>
<td>1000</td>
<td>$4.61 \times 10^{-7}$</td>
<td>$F(x) = (x + (((x * x - x) * (-1.5777)) * (((x + (((x * x) * x - x - 0.8749) \times x) + (((x * x) * x - x) * x) * x) * x) * x) * x) * x)$</td>
</tr>
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</table>

Table 2. The optimal GP-index profile at different generations.
Figure 2. The convergence curves of GP for the refractive index distribution profile optimization.

Figure 3. (a) The optimal GP-index profile and (b) calculated wavelength-dependent reflectivity at normal incidence at 10, 100, 500 and 1000 generations, respectively.

4.29 × 10⁻³% to 4.61 × 10⁻⁷%, that means the average reflectance of AR coatings becomes lower and lower.

For example, when the generations of GP is 10, the optimal GP-index profile for the AR coatings is \( n = n_{\text{low}} + (n_{\text{high}} - n_{\text{low}})(x \ast x) \), in which \( n \) is the refractive index of AR coatings, \( x \) is the relative thickness of AR coatings, \( n_{\text{low}} \) and \( n_{\text{high}} \) are the refractive indices of the incident and substrate media, respectively. The average reflectance of AR coatings is only 4.29 × 10⁻³%. Moreover, when the generations of GP is 100, the optimal GP-index profile for the AR coatings is \( n = n_{\text{low}} + (n_{\text{high}} - n_{\text{low}})((x - 1.5777 \ast (x \ast x \ast x - x) \ast x) \ast x \ast x) \), and its average reflectance of AR coatings has been decreased to 2.14 × 10⁻⁴%. Finally, when the generations of GP is 1000, the optimal GP-index profile for the AR coatings is a very complex nonlinear equation which is clearly expressed in Table 2, and its average reflectance of AR coatings has been decreased to the lowest value of 4.61 × 10⁻⁷%.

The optimal GP-index profile and calculated wavelength-dependent reflectivity at normal incidence at 10, 100, 500 and 1000 generations are presented in Figure 3. From Figure 3(a) it can be seen that the genetic programming algorithm can automatically search through all possible combinations of symbolic expressions with broadband and omnidirectional antireflection characteristics. From Figure 3(b), it can be clearly seen that the wavelength-dependent reflectivity at normal incidence at different generations is also becoming lower and lower. Therefore, the design methodology presented in this paper that uses a genetic programming technique is a quite convenient means to pursue a novel nonlinear refractive index profile with broadband and omnidirectional antireflection characteristics.

Moreover, in order to verify the performance of optimal GP-index profile, we have compared the spectral and angular dependences of the reflectivity for linear profile, cubic profile, quintic profile and optimal GP profile at 1000 generations which are shown in Figure 4(b) and Figure 4(c), respectively.
Figure 4. Different index profiles comparison for graded-index coating. (a) Refractive index profile of a 1000 nm graded-index layer between two dielectric media with \( n_i = 1.6 \) and \( n_s = 2.4 \) for linear-, cubic-, quintic-, and GP-index profiles, respectively. (b) Calculated wavelength-dependent reflectivities for linear-, cubic-, quintic-, and GP-index profiles at incident angle of 40°. (c) Calculated angular-dependent reflectivities for linear-, cubic-, quintic-, and GP-index profiles at a wavelength of 550 nm. The calculation is approximated by using 1,000 sublayers of equal thickness.

Figure 5. Simulated reflection characteristics of AR coatings, (a) linear-index profile, (b) cubic-index profile, (c) quintic-index profile, and (d) GP-index profile as a function of wavelength and incident angle.
Figure 6. Schematic of an 800 nm TiO$_2$/SiO$_2$ graded-index AR coating between air and an AlN substrate with refractive index of \( n = 2.05 \).

Figure 7. Different index profiles comparison for the TiO$_2$/SiO$_2$ graded-index AR coating. (a) Refractive index profile of an 800 nm TiO$_2$/SiO$_2$ graded-index AR coating between air and an AlN substrate with refractive index of \( n = 2.05 \) for linear-, cubic-, quintic-, and GP-index profiles, respectively. (b) Calculated wavelength-dependent reflectivities for linear-, cubic-, quintic-, and GP-index profiles at incident angle of 20°. (c) Calculated angular-dependent reflectivities for linear-, cubic-, quintic-, and GP-index profiles at a wavelength of 632.8 nm which also refer to the literature [21]. The calculation is approximated by using 1,000 sublayers of equal thickness.

Figure 4(a) depicts the refractive index profile of a 1000 nm graded-index layer between two dielectric media with \( n_i = 1.6 \) and \( n_s = 2.4 \) for linear-, cubic-, quintic-, and GP-index profiles, respectively. From the results of Figure 4(b) and Figure 4(c), it can be seen that each graded-index profile exhibits low reflectivity for both transverse electric (TE) and transverse magnetic (TM) polarizations over a broad spectral range, with the GP-index profile having the best performance, with \( R < 1 \times 10^{-6}\% \) for the entire spectrum from 400 nm to 700 nm.

Figures 5(a)–5(d) show a calculated reflectance of linear-index profile, cubic-index profile, quintic-
index profile and GP-index profile respectively, as a function of wavelength and incident angle. The GP-index profile shows a significant reduction in reflectance over a wide range of incident angles and wavelengths in comparison with linear profile, cubic profile and quintic profile. The calculated average reflectance \( R_{\text{ave}}(\lambda, \theta) \), over the wavelength range of 400–700 nm and incident angles from 0° to 90°, is summarized in Figure 5. Conventional linear profile, cubic profile and quintic profile can achieve a low average reflectance \( R_{\text{ave}}(\lambda, \theta) \) of 8.09 × 10\(^{-3}\)%, 3.29 × 10\(^{-4}\)% and 4.35 × 10\(^{-5}\)% respectively. However, the proposed GP-index profile in this paper can obtain an extremely low average reflectance \( R_{\text{ave}}(\lambda, \theta) \) of 4.61 × 10\(^{-7}\)% which is obviously superior to the average reflectance of linear profile, cubic profile and quintic profile. That means, Fresnel reflection almost can be eliminated by the optimal GP-index profile for omnidirectional incidence over a broad wavelength range.

4. ROBUSTNESS VERIFICATION OF GP-INDEX PROFILE

To further verify the robustness and universality of the optimal GP-index profile proposed in this paper, we have compared the broadband and omnidirectional antireflection characteristics of linear profile, cubic profile, quintic profile and optimal GP profile at 1000 generations for another TiO\(_2\)/SiO\(_2\) graded-index AR coating which was proposed in literature [21].

Figure 6 depicts the schematic of an 800 nm TiO\(_2\)/SiO\(_2\) graded-index AR coating between air and an AlN substrate with refractive index of \( n = 2.05 \) which refer to the literature [21].

Figure 7 presents the different index profiles comparison for the TiO\(_2\)/SiO\(_2\) graded-index AR coating. Figure 7(a) depicts the refractive index profile of an 800 nm TiO\(_2\)/SiO\(_2\) graded-index AR coating between air and a AlN substrate with refractive index of \( n = 2.05 \) for linear-, cubic-, quintic-, and GP-index profiles, respectively. From the results of Figure 7(b) and Figure 7(c), it can be seen that the GP-index profile still has the best performance for both transverse electric (TE) and transverse magnetic (TM) polarizations for the entire spectrum from 300 nm to 1400 nm. And the reflectivity of GP-index profile is far lower than the conventional linear, cubic and quintic profiles for any wavelength.

Now, let’s move on to the next section, which will discuss the simulation results of the reflection characteristics of the TiO\(_2\)/SiO\(_2\) graded-index AR coating.
range or incident angle.

Figures 8(a)–8(d) show a calculated reflectance of linear-index profile, cubic-index profile, quintic-index profile and GP-index profile for the TiO$_2$/SiO$_2$ graded-index AR coating, as a function of wavelength and incident angle. The GP-index profile still shows a significant reduction in reflectance over a wide range of incident angles and wavelengths in comparison with linear profile, cubic profile and quintic profile. The calculated average reflectance $R_{ave}(\lambda, \theta)$, over the wavelength range of 300–1400 nm and incident angles from 0° to 90°, is summarized in Figure 8.

Conventional linear profile, cubic profile and quintic profile can achieve a low average reflectance $R_{ave}(\lambda, \theta)$ of 8.23%, 7.96% and 8.25%, respectively. We note that the performance of quintic profile is worst among three conventional profiles which only obtains an average reflectance of 8.25% because of the nonoptimal choice in AR coating thickness, or the nonoptimal chosen wavelength range. However, the proposed GP-index profile in this paper can achieve a lowest average reflectance $R_{ave}(\lambda, \theta)$ of 7.74%. That means, the proposed GP-index profile has better robustness and universality, and it still has the best broadband and omnidirectional antireflection characteristics for the TiO$_2$/SiO$_2$ graded-index AR coating.

5. CONCLUSION

In conclusion, to eliminate the average reflectance of AR coatings to the greatest extent, a genetic programming (GP) algorithm is proposed to design and optimize the graded refractive index distribution profile for broadband omnidirectional antireflection coatings. The proposed GP-index profile in this paper can obtain an extremely low average reflectance of $4.61 \times 10^{-7}\%$ over a wide range of incident angles and wavelengths which is obviously superior to the average reflectance of $8.09 \times 10^{-3}\%$, $3.29 \times 10^{-4}\%$ and $4.35 \times 10^{-5}\%$ for linear profile, cubic profile and quintic profile. That means, Fresnel reflection almost can be eliminated by the optimal GP-index profile for omnidirectional incidence over a broad wavelength range.

Moreover, to further verify the robustness and universality of the optimal GP-index profile proposed in this paper, we have compared the broadband and omnidirectional antireflection characteristics of linear profile, cubic profile, quintic profile and optimal GP profile for another TiO$_2$/SiO$_2$ graded-index AR coating. It is demonstrated the proposed GP-index profile has better robustness, and it still has the best broadband and omnidirectional antireflection characteristics for the TiO$_2$/SiO$_2$ graded-index AR coating.

Therefore, we have proven, with the aid of numerical modeling, that the proposed GP-index profile is obviously superior to the conventional linear profile, cubic profile and quintic profile, and the design methodology presented in this paper that uses a genetic programming technique is a quite convenient means to pursue an optimal nonlinear refractive index profile with broadband and omnidirectional antireflection characteristics.

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