

# Genetic algorithm for design of reflective filters: application to $\text{Al}_x\text{Ga}_{1-x}\text{N}$ based Bragg reflectors

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## ABSTRACT

A genetic algorithm (GA) with adaptive mutations has been employed for the design of Bragg reflectors. The algorithm enables three different design types a) composition and thickness of two layers are chosen and the pair is repeated b) two compositions are chosen for the two alternating materials, and thickness of each layer is optimized c) composition and thickness of each layer are optimized. In all cases, the wavelength and composition dependence of the index of refraction is taken into account. Also, it is possible to impose constraints on the composition difference of the neighbouring layers, either with a penalty function or with narrowing the boundaries for possible compositions. This feature is important because the large lattice mismatch between GaN and AlN can cause poor surface morphology, so measured reflectivity would be lower than the calculated one due to the surface roughness. The algorithm enables finding the optimal design for two chosen incident and final media, and it is capable of taking into account the existence of a finite, optically thick substrate. We have investigated two systems: air/sapphire/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$  reflector/GaN and GaN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /air.

**Keywords:** Genetic algorithms, group-III nitrides

## 1. INTRODUCTION

Group III nitride devices have recently attracted much attention for applications in optoelectronic devices operating in the blue-green and ultraviolet part of the spectrum.<sup>1,2</sup> Among other devices, realization of an optically pumped vertical cavity surface emitting laser (VCSEL) has been reported.<sup>3,4</sup> VCSELs require highly reflective mirrors on both sides to achieve lasing due to short cavity length. Therefore, highly reflective group III nitride based Bragg reflectors are necessary for GaN based VCSELs. GaN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ,  $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$  and GaN/AlN Bragg reflectors have been reported<sup>5-9</sup>

In order to achieve high reflectivity, a multilayer consisting of alternating quarter-wave layers with high (H) and low (L) refractive indices should contain a large number of HL pairs, or have large difference between H and L refractive index. However, a number of layer pairs is limited due to large lattice mismatch between GaN and AlN. Lattice mismatch causes strains in the layer which can result in poor surface morphology. For the heterostructures with 20 or more periods, lattice mismatch should be below or equal 1%.<sup>5</sup> If the lattice mismatch was larger, surface quality of the layers would be poor, which would result in lower reflectivity due to scattering losses. AlN/GaN multilayers, which have the largest difference between refractive indices of all  $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$  combinations, clearly do not satisfy the conditions for growing large number of layer pairs. The largest reported number of layer pairs in AlN/GaN reflectors is 20.5, and achieved reflectivity is 95% at 392.5 nm.<sup>9</sup> 14 pair GaN/AlN reflector, which has been grown in such a manner that surface morphology is improved, has a reflectivity peak at 456 nm of only 88%.<sup>6</sup> Better results can be achieved with a large number of layers with smaller composition difference. Highly reflective (96±2%) filters with 35 GaN/ $\text{Al}_{0.34}\text{Ga}_{0.66}\text{N}$  pairs have been reported.<sup>8</sup> Therefore, the number of layer pairs and the composition difference between the layers should be carefully chosen to achieve optimal reflectivity.

In this work we propose a genetic algorithm (GA) for the design of  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  based reflectors. The algorithm enables three different design types a) composition and thickness of two layers are chosen and the pair is repeated b) two compositions are chosen for the two alternating materials, and thickness of each layer is optimized c) composition and thickness of each

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layer are optimized. The GA approach is completely independent on the nature of the multilayer, as well as the incident and the substrate media. Also, it is straightforward to impose constraints on various properties of the multilayer, such as the refractive index difference of neighbouring layers, and change the design objective by manipulating the objective function. GAs have been employed in thin film filter design, for filters containing dielectric<sup>10,11</sup> or dielectric and metallic layers.<sup>12</sup> In applying GAs to semiconductor reflective filter design it is possible to take into account the dependence of both the real and imaginary parts of the index of refraction on wavelength, as well as impose constraints to ensure that necessary design requirements have been met. GAs represent global optimization methods which mimic the concept of evolution. GAs apply evolution mechanisms, such as selection, reproduction (which includes choice of parents and crossover to produce offspring) and mutation, to a set of possible solutions called population. Each individual member of the population is a vector of variables called a chromosome. Each variable is called a gene. Chromosomes are characterized by fitness, which represents a quantitative measure of how well a chromosome satisfies set design specifications. In this work, fitness is inversely proportional to the sum of objective function and penalty function(s). Objective function is defined as a sum of squared discrepancies between the calculated and desired reflectance curve, while the penalty functions are defined according to design limitations, such as maximal allowed composition difference between the neighbouring layers. Fitness of a chromosome determines the probability that a chromosome will survive unchanged or give offspring in the next generation. After a number of generations, optimal solution should be reached.

Since GA based thin film filter design procedures have several advantages over classical design procedures,<sup>13</sup> in this work we have used the elite genetic algorithm with adaptive mutations for the design of  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  based reflectors. The algorithm employs floating-point scheme for layer thickness and composition, which are the values to be optimized. By changing the composition  $x$ , the index of refraction of the layer is optimized. We present calculations for reflectors designed for the peak reflectance at 390 nm and bandwidth of 20 nm. We have investigated two systems: air/sapphire/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$  reflector/GaN and GaN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /air, where GaN is incident medium. For the first structure, we disregard the thin GaN (or AlN) low-temperature buffer layer. It has been shown that the existence of a low-temperature buffer layer improves the surface quality of a nitride film grown above the buffer layer.<sup>14,15</sup> We have not taken this layer into account in our calculations, since the exact dependence of the index of refraction of the buffer layer is not known. The buffer layer is usually very thin and its refractive index is lower than the refractive index of wurtzite GaN,<sup>16</sup> so existence of a buffer layer should not significantly compromise accuracy of our calculations.

## 2. DESCRIPTION OF THE ALGORITHM

In order to implement a GA, we must define the coding scheme, initial population generation, and selection, crossover and mutation operators. In this work we have used elite genetic algorithm with adaptive mutations (EGAAM).<sup>17</sup> Floating-point coding scheme<sup>17-19</sup> has been employed. Each layer is characterized with two real numbers, alloy composition and layer thickness. In this coding scheme, each gene has the value of the corresponding variable  $p(k)$ ,  $k=1, n_v$ , where  $n_v$  is the number of variables. The number of variables differs for three design procedures. In the design procedure c), composition and thickness of each layer are chosen independently, and the total number of variables is equal  $2 \times n_l$ , where  $n_l$  is the number of layers. In design procedure b), two materials are used while layer thickness of each layer is still determined independently, so that the number of variables is  $n_l + 2$ , for two layer compositions and  $n_l$  layer thickness parameters. For design procedure a), the algorithm chooses only alloy composition and layer thickness for two layers, which are repeated required number of times, so that the number of variables is 4 regardless of the number of layers. This design procedure is the closest to the conventional quarter-wave design. The advantage of this procedure over the conventional design is that the constraints can be introduced, and optimal design found within given constraints. The values of variables in the initial population are in all cases generated according to the equation<sup>17</sup>

$$p(k) = p_l(k) + (p_u(k) - p_l(k)) \times r \quad , \quad (1)$$

where  $r$  is a random number  $r \in [0,1]$ , and  $p_l(k)$  and  $p_u(k)$  are initially set lower and upper boundary, respectively. In such a manner, confinement of the variables in the specified domain is achieved in order to insure that variables have physical meaning, i.e. that all the thickness values are positive and all the compositions  $0 \leq x \leq 1$ .

EGAAM employs elitist selection mechanism.<sup>20-22</sup> In this selection mechanism,  $P_s$  percent of the strings in the current population enter the next population unchanged, while  $P_c$  percent of the strings in the new population are generated by crossover between the parent strings.  $P_s$  and  $P_c$  are initially specified values. Parent strings on which crossover is performed

are chosen fitness proportionally. The probability of a string having offspring in the next generation is inversely proportional to<sup>17</sup>

$$F(i) = \frac{f(i)}{\sum_i f(i)} , \quad (2)$$

where  $f(i)$  is the fitness value of  $i$ -th string.

Operation of crossover exchanges subsets of elements between two parent strings. If the subsets consist of adjacent elements, it is an “ordered combination” crossover, while in “uniform combination” crossover each element is randomly chosen.<sup>23</sup> EGAAM employs “uniform combination” crossover, with a number of elements to be exchanged randomly generated at each crossover operation.<sup>17</sup> After the number of elements to be exchanged has been generated (which is always greater than the specified minimal number of elements), random integers determining positions of elements to be exchanged are generated and elements on those positions are swapped.

Mutation ensures that the population diversity is maintained, thus preventing quick convergence to a local minimum. If the mutation probability is too large, mutation no longer improves the performance of the algorithm, since it enables losses of genetic information which can cause poor convergence.<sup>24</sup> EGAAM employs adaptive mutation concept<sup>17</sup> in order to overcome the phenomenon that real-coded GA can be blocked from further progress.<sup>25,26</sup> In adaptive mutation scheme,  $P_m$  percent of completely new strings are introduced in every generation. The new strings are generated in the same way as during initial population generation, but within narrowed boundaries to provide that more strings are generated in the area where a solution is expected. The boundaries are narrowed according to equations<sup>17</sup>

$$p_{new-u}(k) = p_{old-u}(k) - c(p_{old-u}(k) - \mu(k)) , \quad (3)$$

$$p_{new-l}(k) = p_{old-l}(k) + c(\mu(k) - p_{old-l}(k)) , \quad (4)$$

where  $\mu(k)$  is the average value of parameter  $p(k)$  in the current population, and  $c$  is a predetermined positive number  $c < 1$ . To prevent excessive narrowing of the boundaries, lower boundary was limited to be less than maximal allowed lower boundary, and upper boundary was limited to be greater than minimal allowed upper boundary.

The objective function represents a measure of the quality of the obtained solution. To achieve the desired reflectance dependence on the wavelength  $\lambda$ , we have used the following objective function

$$F = \left\{ \sum_{i=1}^{n_p} (R_c - R_d)^2 \exp\left(-\frac{(\lambda - \lambda_0)^2}{2\sigma^2}\right) \right\} + \Delta , \quad (5)$$

where  $n_p$  is the number of points in which we calculate the reflectance  $R_c$ ,  $R_d$  is the desired reflectance, and  $\lambda_0$  is the wavelength where peak reflectivity should be achieved.  $\Delta$  is the penalty function, whose value is set to zero if the composition difference constraints are satisfied, or set to a specified value  $10 \leq \Delta \leq 100$  if the composition difference between adjacent layers is larger than the required value. The desired reflectance is equal to 1.0 in the range  $[\lambda_0 - \Gamma, \lambda_0 + \Gamma]$  where  $\Gamma$  is the half-width of reflectance peak, and equal to zero outside that range. The exponential factor in Eq. (5) provides enhancement of the peak at  $\lambda_0$ .

We shall briefly give the theoretical background of transport of electromagnetic wave through a series of layers with the complex index of refraction  $N_i = n_i - ik_i$  and thickness  $d_i$ , placed between the incident and substrate media with the index of refraction values  $n_0$  and  $N_s$ . The equations are given for the case of perpendicular polarization only, since the procedure for parallel polarization is completely analogous. In the case of one dielectric layer, electric and magnetic fields of the incident ( $E_I, H_I$ ) and transmitted ( $E_{II}, H_{II}$ ) waves are related in a following manner<sup>27,28</sup>

$$\begin{bmatrix} E_I \\ H_I \end{bmatrix} = M \cdot \begin{bmatrix} E_{II} \\ H_{II} \end{bmatrix}, \quad (6)$$

where

$$M = \begin{bmatrix} \cos(k_0 h) & i \frac{1}{Y_i} \sin(k_0 h) \\ i Y_i \sin(k_0 h) & \cos(k_0 h) \end{bmatrix}. \quad (7)$$

Time dependence of the electric field has the form  $\exp(i\omega t)$ ,  $k_0 = 2\pi/\lambda$  is the wave number of the incident electromagnetic wave,  $h = N_i d \cos\theta_i$ ,  $\theta_i$  is the angle of the electric field within the layer, and  $Y_i$  is given by

$$Y_i = \sqrt{\frac{\varepsilon_0}{\mu_0}} N_i \cos\theta_i. \quad (8)$$

In the case of  $L$  layers between the incident and substrate media, we can assign to each layer the matrix in the form of Eq. (7). The connection between electric and magnetic fields before  $(E_I, H_I)$  and after  $(E_{L+1}, H_{L+1})$  the multilayer structure is described by

$$\begin{bmatrix} E_I \\ H_I \end{bmatrix} = \left( \prod_{i=1}^N M_i \right) \cdot \begin{bmatrix} E_{L+1} \\ H_{L+1} \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \cdot \begin{bmatrix} E_{L+1} \\ H_{L+1} \end{bmatrix}. \quad (9)$$

Fresnel coefficients are then given with

$$r = \frac{Y_0 \cdot m_{11} + Y_0 \cdot Y_s \cdot m_{12} - m_{21} - Y_s \cdot m_{22}}{Y_0 \cdot m_{11} + Y_0 \cdot Y_s \cdot m_{12} + m_{21} + Y_s \cdot m_{22}}, \quad (10)$$

$$t = \frac{2 Y_0}{Y_0 \cdot m_{11} + Y_0 \cdot Y_s \cdot m_{12} + m_{21} + Y_s \cdot m_{22}}, \quad (11)$$

where  $n_0$  and  $N_s$  are the index of refraction values of the incident and substrate medium, respectively, while  $Y_0$  and  $Y_s$  are the corresponding admittance values defined in the same manner as the  $Y_i$  in equation (8). Ratios of the intensities of the transmitted and incident waves and the reflected and incident waves are described by the transmittance  $T = t t^* \text{Re}(N_s \cos\theta_s) / (n_0 \cos\theta_0)$  and reflectance  $R = r r^*$ , where  $r^*$  and  $t^*$  are the complex conjugated values of the Fresnel coefficients  $r$  and  $t$ . In the structure air/sapphire/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$  reflector/ $\text{GaN}$ , since we have an optically thick, transparent substrate, it is necessary to introduce the correction for the reflection from the sapphire-air surface. The reflectance and transmittance at sapphire-air surface in case of normal incidence are  $R_s = ((n_s - 1) / (n_s + 1))^2$  and  $T_s = 4n_s / (n_s + 1)^2$ . The corrected values for reflectance and transmittance<sup>29</sup> are described with:

$$\bar{R} = R + \frac{T T' R_s}{1 - R' R_s}, \quad (12)$$

$$\bar{T} = \frac{T T_s}{1 - R' R_s}, \quad (13)$$

where  $R'$  and  $T'$  are reflectance and transmittance from the back side of a multilayer.

The index of refraction of  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  as a function of wavelength (energy  $\hbar\omega$  (eV) = 1239.85/ $\lambda$  (nm)) and composition can be described with a simple expression in the spectral region of interest<sup>30</sup>

$$n^2(\omega) = C(x) + A(x) y^{-2} \left( 2 - \sqrt{1+y} - \sqrt{1-y} \right), \quad y = \frac{\hbar\omega}{E_g}, \quad (14)$$

$$A(x) = 3.17\sqrt{x} + 9.98, \quad (15)$$

$$C(x) = -2.2x + 2.66, \quad (16)$$

$$E_g(x) = E_g(\text{GaN})(1-x) + E_g(\text{AlN})x - bx(1-x) \quad , \quad (17)$$

where  $E_g(\text{GaN})=3.42$  eV,  $E_g(\text{AlN})=6.13$  eV and  $b=1.3$  eV. However, in order to take into account the absorption in the spectral region of interest for alloys  $0 \leq x \leq 0.4$  it is convenient to rewrite the Eq. (14), with  $N^2(\omega) = \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ , as:<sup>31</sup>

$$\varepsilon_1(\omega) = C(x) + A(x)y^{-2}\left(2 - \sqrt{1+y} - \sqrt{1-y}H(1-y)\right), \quad (18)$$

$$\varepsilon_2(\omega) = A(x)y^{-2}\sqrt{y-1}H(y-1), \quad (19)$$

where  $H(x) = 1, x \geq 0$  and  $H(x)=0, x<0$ . The real and imaginary part of the index of refraction are then readily calculated from the formulae  $n = \left[0.5(\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2})\right]^{1/2}$  and  $k = \left[0.5(-\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2})\right]^{1/2}$ . The optical constants of sapphire in the spectral region of interest can be described with  $k_s=0.0$  and  $n_s=1.752+5497.26/\lambda^2$ , which describe well the tabulated data.<sup>32</sup>

### 3. RESULTS AND DISCUSSION

If no constraints are imposed, the algorithm will produce an alternating sequence of GaN/AlN layers for all three design methods a), b), and c). This is because GaN and AlN have the largest possible difference in refractive indices, and therefore the calculated reflectivity of a GaN/AlN reflector would be the highest for a given number of layers. However, due to practical limitations in the growth of GaN/AlN reflectors, we will limit our discussion to the cases where the composition difference between adjacent layers is  $\leq 0.5$ . We compare the calculated reflectance of conventionally designed reflectors consisting of alternating layers of  $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$  with layer thickness determined with  $d_i=\lambda_0/4n_i$ , where  $n_i$  is the refractive index of the layer.

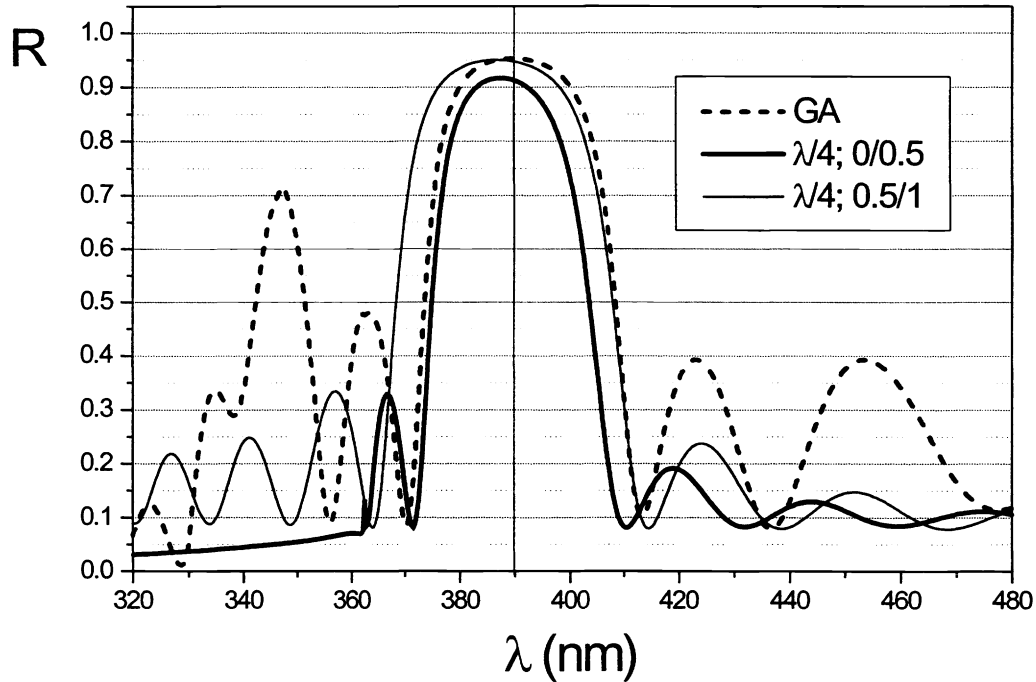


Fig. 1 The reflectance of a 30 layer reflector for the structure air/sapphire/reflector/GaN. Dashed line denotes GA optimized design with composition difference  $\leq 0.5$ , while thick and thin solid lines denote  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}/\text{GaN}$  and  $\text{AlN}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$  quarter-wave reflectors, respectively.

In Fig. 1, dashed line denotes GA optimized design with method c) and composition difference  $\leq 0.5$  for structure air/sapphire/reflector/GaN, while thick and thin solid lines denote  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}/\text{GaN}$  and  $\text{AlN}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$  quarter-wave

reflectors, respectively. Fig. 2 shows the obtained results for the structure GaN/reflector/air. In all cases, calculations for 30 layers are presented. Light is incident from GaN. It can be clearly observed that the value of the reflectance peak in the conventional design depends on the composition of the layers and not only on the composition difference between the layers. Therefore, although GA optimized design using method a) produces a sequence of  $\lambda/4$  alternating layers similar to the conventional design, the important advantage of this method is that it chooses automatically which compositions should give the highest reflectance for given composition difference.

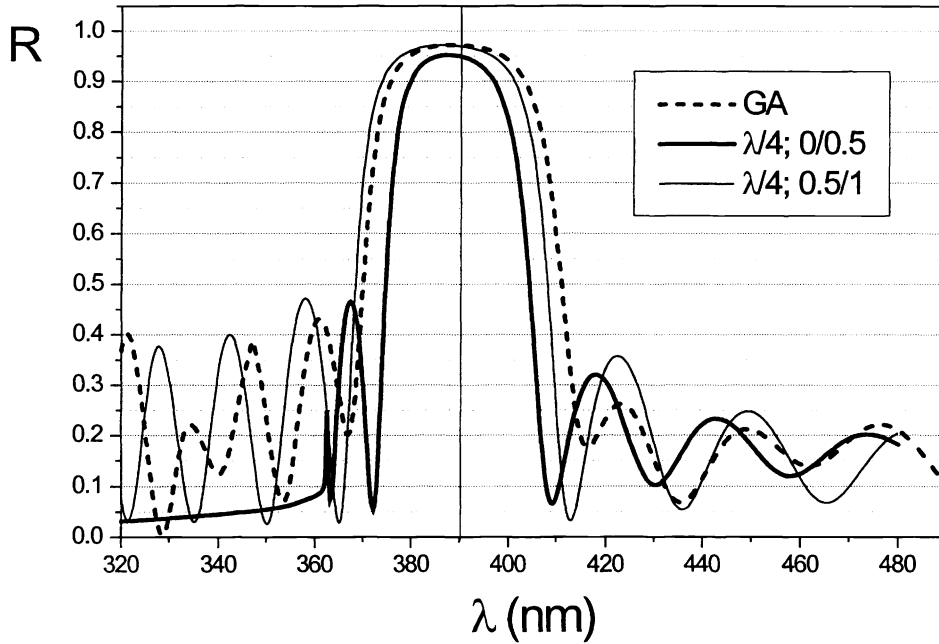


Fig. 2 The reflectance of a 30 layer reflector for the structure GaN/reflector/air. Dashed line denotes GA optimized design with composition difference  $\leq 0.5$ , while thick and thin solid lines denote  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}/\text{GaN}$  and  $\text{AlN}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$  quarter-wave reflectors, respectively.

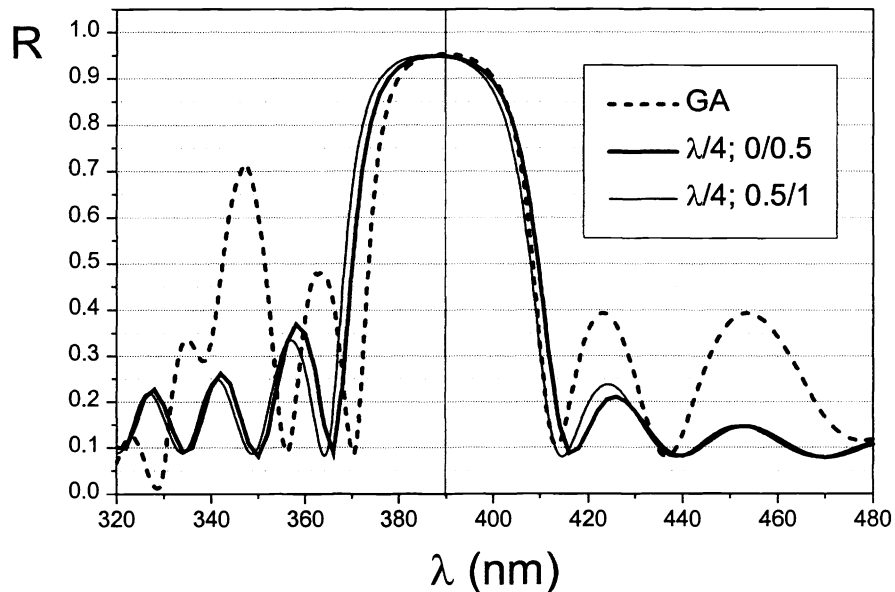


Fig. 3 The reflectance of a 30 layer reflector for the structure GaN/reflector/air. Dashed line denotes GA optimized design with composition difference  $\leq 0.5$ , design method c), while thick solid line denotes results of method b), and thin solid lines denotes  $\text{AlN}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$  quarter-wave reflectors.

In a simple case, such as GaN/reflector/air structure, design method a) should be clearly preferred as the least computationally extensive method, since it involves only four variables. However, for structures such as air/sapphire/reflector/GaN methods b) and c) have an advantage over method a). In those two methods thickness of each layer is chosen independently, so that it is possible to compensate for the optical path within the substrate. Therefore, methods b) and c) would give an optimized design with a reflectance peak at the desired position, while the conventional design and GA optimized design using method a) would produce slightly shifted peak. Also, design method c) has more degrees of freedom than design method b) and hence it should be employed if there are additional layers between the sapphire substrate and  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  reflector. For the structure air/sapphire/reflector/GaN, both design methods b) and c) have similar performance, as can be observed in Fig. 3. However, design method c) produces no shift of the desired peak reflectance, where in the design method b) there is still a shift, though smaller than in the conventional design.

#### 4. CONCLUSION

We have presented genetic algorithm based method for design of  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  reflectors. We have employed three possible design procedures: a) composition and thickness of two layers are chosen and the pair is repeated, b) two compositions are chosen for the two alternating materials, and thickness of each layer is optimized, and c) composition and thickness of each layer are optimized, to the design of reflectors for the structures air/sapphire/reflector/GaN and GaN/reflector/air. All design procedures take into account the wavelength dependence of the complex index of refraction of each layer in the structure, and all have the feature of enforcing the limit to the composition difference of adjacent layers via penalty function. For simple structures, such as GaN/reflector/air, all design procedures have similar performance, while in the presence of substrate and/or additional layers methods b) and c) should be preferred.

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