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Light-extraction enhancement for light-emitting diodes: a firefly-inspired structure refined by the genetic algorithm

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ABSTRACT

The efficiency of light-emitting diodes (LED) has increased significantly over the past few years, but the overall efficiency is still limited by total internal reflections due to the high dielectric-constant contrast between the incident and emergent media. The bioluminescent organ of fireflies gave incentive for light-extraction enhancement studies. A specific factory-roof shaped structure was shown, by means of light-propagation simulations and measurements, to enhance light extraction significantly. In order to achieve a similar effect for light-emitting diodes, the structure needs to be adapted to the specific set-up of LEDs. In this context simulations were carried out to determine the best geometrical parameters.

In the present work, the search for a geometry that maximizes the extraction of light has been conducted by using a genetic algorithm. The idealized structure considered previously was generalized to a broader variety of shapes. The genetic algorithm makes it possible to search simultaneously over a wider range of parameters. It is also significantly less time-consuming than the previous approach that was based on a systematic scan on parameters. The results of the genetic algorithm show that (1) the calculations can be performed in a smaller amount of time and (2) the light extraction can be enhanced even more significantly by using optimal parameters determined by the genetic algorithm for the generalized structure. The combination of the genetic algorithm with the Rigorous Coupled Waves Analysis method constitutes a strong simulation tool, which provides us with adapted designs for enhancing light extraction from light-emitting diodes.

Keywords: light-emitting diode (LED), firefly, light extraction, optimization, genetic algorithm

1. INTRODUCTION

The light-extraction efficiency (LEE) of light-emitting devices is fundamentally limited by the high dielectric-constant contrast between the incident material and the emergent material. Various approaches are considered in order to increase the extraction of light from high dielectric-constant materials, including plasmonics, interface structuring and alteration of the light-emitting material by encapsulation.¹⁻⁴ In the present paper, we will describe a theoretical approach that enables the determination of optimal parameters in order to achieve high extraction efficiencies.

A previous study⁵ on the morphology of the bioluminescent organ of fireflies showed that the cuticle surface presents a specific jagged scales pattern, which turns out to increase significantly the LEE in comparison to a planar surface. This specific structure is used as a starting point to enhance the light-extraction efficiency of a blue light-emitting diode. Several parameters of the structure are varied using the genetic algorithm and the effect on the light-extraction efficiency is analyzed.

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Our objective is to maximize the light-extraction efficiency η , which is defined as the ratio between the intensity I_{trans} of the light extracted into free space and the intensity I_{inc} of the light emitted in the active material (Eq. 1).

$$\eta(\%) = \frac{I_{\text{trans}}}{I_{\text{inc}}} \times 100 \quad (1)$$

To quantify the increase in LEE, we define the light-extraction efficiency enhancement $\Delta\eta$ as the relative increase of the LEE of the structured device η_{struct} , when comparing with the LEE of the reference model η_{ref} (Eq. 2). The reference model consists in a light-emitting material with the same dielectric constant as the structured device, but terminated by a planar interface.

$$\Delta\eta = \frac{\eta_{\text{struct}} - \eta_{\text{ref}}}{\eta_{\text{ref}}} \times 100 \quad (2)$$

2. FORMER RESULTS

The surface of the cuticle of fireflies is characterized by jagged scale structures, which influence the LEE.⁵ The mean period of these structures is about $10 \mu\text{m}$ and the height is about $3 \mu\text{m}$ (see Fig 1). Simulations were carried out by using a Rigorous Coupled Waves Analysis method. They show that the LEE enhancement reaches the value of $\Delta\eta = 45\%$, when comparing with a planar surface. The question then arises whether similar, but slightly different, structures could be even more efficient.

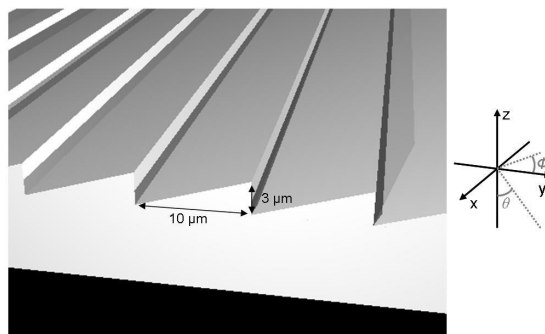


Figure 1. Schematic representation of the jagged scales found on the firefly cuticle.

A closer study of the jagged scale structure was carried out by varying the geometrical parameters of this structure, i.e. the period p and the height h . We also investigated related structures, i.e. a triangle, a pyramid and a cone, by a similar variation of p and h . The four structures considered in this study are represented in Fig. 2.

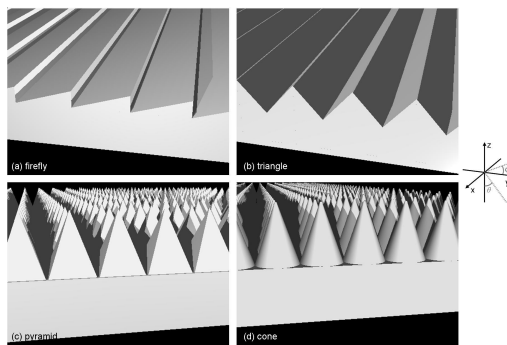


Figure 2. Different shapes considered in the case of the firefly. Two-dimensional shapes: (a) jagged scales and (b) triangles and three-dimensional shapes: (c) pyramids and (d) cones.

Parameter optimization in this previous study was actually carried out by a systematic scan on p and h . The step considered for the variations of p and h was $1 \mu\text{m}$. The results of this study - published by Bay *et al.*⁶ - led

to the conclusion that the jagged scale structure is the most efficient, as it provides a LEE enhancement as high as $\Delta\eta = 58\%$ when considering a period $p=8\mu\text{m}$ and a height $h=7\mu\text{m}$. Fig. 3(b) shows the profile associated with these optimal parameters.

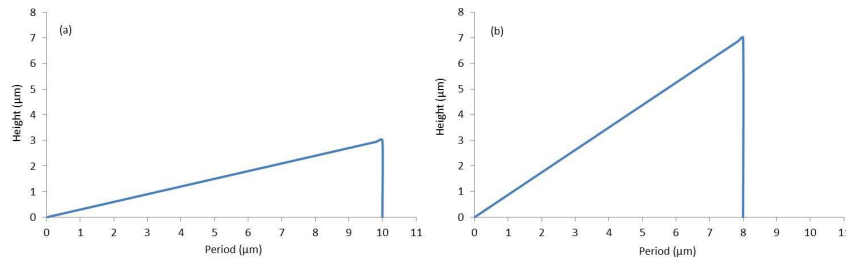


Figure 3. Profiles of the simulated structures in the firefly case. (a) Period $p=10\mu\text{m}$ and height $h=3\mu\text{m}$ found on the firefly (see Fig. 1). (b) Period $p=8\mu\text{m}$ and height $h=7\mu\text{m}$ after search for the highest LEE.

This approach was very time-consuming. The simulations have been done for structures varying in period p and height h from $1\mu\text{m}$ to $15\mu\text{m}$, by steps of $1\mu\text{m}$. The number of structures that were evaluated was large: $15 \times 15 = 225$ for each configuration (jagged scales, triangles, pyramids and cones), giving a total of 900 evaluations. Considering that one evaluation took typically four hours, the total computing time was 3600 hours or 150 days. Another disadvantage of this approach is that the variation step was quite coarse. The probability to miss a more efficient structure is high.

This significant increase in the LEE of a high dielectric-constant light-emitting material led to a closer investigation of the jagged scale structure for fabrication on a gallium-nitride (GaN)-based light-emitting diode. The emission wavelength is 425 nm. In the case of a light-emitting diode, the dielectric constant of the emitting material is even higher than in the case of organic bioluminescent organs and the light extraction for a planar interface is therefore very limited. A Ni/Au current spreading layer is added on top of the light-emitting material for functioning purposes of the LED. The light-extraction efficiency for such a GaN-based LED terminated by a planar surface has been estimated to be $\eta_{\text{ref}} = 3.7\%$ only.

Former simulations, in which the period p and the height h of the jagged scales structure were varied by steps of $1\mu\text{m}$, show that the LEE can be enhanced up to $\eta_{\text{struct}} = 5.7\%$. The optimal parameters were found to be $p=5\mu\text{m}$ and $h=6\mu\text{m}$. When comparing with a system terminated by a planar surface, the LEE enhancement is $\Delta\eta = 54\%$.⁷ In this case, $15 \times 15 = 225$ different structures were evaluated when exploring the jagged scale shape.

3. GENETIC ALGORITHM

Let us consider a different approach for the parameter optimization. The function to be optimized is the light-extraction efficiency η of a light-emitting diode, as defined in the Introduction. This function has a number n of variable physical parameters x_i , where $x_i \in [x_i^{\min}, x_i^{\max}]$ with a specific granularity of Δx_i . We approach this optimization problem by using this time a genetic algorithm. This approach will provide a globally maximized function f , defined by a specific set of parameters x_i .

Each of the structural parameters x_i is represented by a gene, which consists of a string of n_i bits (0 or 1). The corresponding value of x_i is given by

$$x_i = x_i^{\min} + \langle \text{gene} \rangle_i \frac{x_i^{\max} - x_i^{\min}}{2^{n_i} - 1}, \quad (3)$$

where $\langle \text{gene} \rangle_i$ is the value coded by the i^{th} gene in Gray binary coding.⁸ The length n_i of each gene is chosen so that $(x_i^{\max} - x_i^{\min})/(2^{n_i} - 1) \leq \Delta x_i$. The juxtaposition of the n genes used for the representation of each parameter is called *DNA*. The optimal solution is searched for by working on the DNA representation of the structural parameters.

We work with a population of $n_{\text{pop}}=100$ individuals. Each individual has its own DNA and is therefore representative of a given set of structural parameters. The initial population consists of random individuals.

The first step is to evaluate the fitness, i.e. the light-extraction efficiency, of these 100 individuals. Out of these 100 individuals, $n_{\text{pop}}/2$ individuals (the *parents*) are chosen by a random selection procedure that takes into account the actual fitness of each individual. Individuals with a higher fitness have a higher chance to be selected. Each individual can be selected several times. This enables the best individuals to progressively dominate the population. We define the mean value of the fitness f_{mean} as the average fitness value of the whole population. The best fitness f_{best} corresponds to the highest LEE achieved in the population.

The parents are transferred to the next generation. For each pair of parents, two *children* are created either by (a) a one-point crossover of the parent's DNA, or by (b) a simple replication of the parent's DNA. These events occur with a probability of 90% and 10%, respectively. The one-point crossover of the parent's DNA is intended to explore new solutions, whereas the transmission of unchanged individuals to the next generation contributes to the conservation of good solutions.

We finally introduce random mutations in the children's DNA. At a high rate of mutations ($> 5\%$ for each bit) the exploration is very random and convergence is unreasonably slow. For a low rate of mutations ($< 0.1\%$) the convergence of the genetic algorithm tends to be too fast and a local maximum may be found instead of the global maximum.

The three steps - selection, crossover/replication and mutation - are repeated for each new generation. Elitism is implemented in order to ensure that the best solution is not lost when going from one generation to the next. The 10% least efficient individuals in terms of fitness are replaced by random individuals. This is done again to ensure a good exploration of the entire parameter space.

The genetic similarity s represents the fraction of bits in the population whose value is the same as for the best individual. The genetic similarity provides a useful monitoring of the population dynamics. It is defined by

$$s = \frac{1}{n_{\text{bits}}(n_{\text{pop}} - 1)} \sum_{\substack{k=1 \\ k \neq k_{\text{best}}}}^{n_{\text{pop}}} \sum_{i=1}^{n_{\text{bits}}} \delta_{b_i[k], b_i[k_{\text{best}}]}, \quad (4)$$

where $n_{\text{bits}} = \sum_{i=1}^n n_i$. $b_i[k]$ refers to the i^{th} bit in the DNA of the k^{th} individual. k_{best} refers to the best individual in the current population. At the beginning, the genetic similarity s typically takes a value of 0.5, indicating a random population. If $s = 1$, the population is completely dominated by the best individual.

Three different criteria are used to terminate the genetic algorithm: (a) the improvement of the best fitness f_{best} was less than 0.5% over a determined number of generations, (b) the genetic similarity s reached a value over 90% over a determined number of generations or, (c) $s \geq 1 - m$, m being the mutation rate, and $f_{\text{mean}} \geq 0.85 \times f_{\text{best}}$.

4. APPLICATION OF THE GENETIC ALGORITHM TO THE FIREFLY INSPIRED STRUCTURE

In this section we describe the results provided by the genetic algorithm when applied to two sets of parameters. In a first approach, the period p , the height h and the dielectric constant $\varepsilon_{\text{form}}$ of the structure used for the surface texturation of the LED were varied. The dielectric constant of the emitting material was kept constant. In a second approach, three parameters were varied in addition to the period p and the height h : the position of the apex c , the concavity of the left edge α_{left} and the concavity of the right edge α_{right} .

The geometry of the structure is defined by

$$h(x) = \begin{cases} h \times \left[1 - \frac{(c.p-x)^{\alpha_{\text{left}}}}{(c.p)^{\alpha_{\text{left}}}} \right] & \text{when } 0 \leq x \leq c.p \\ h \times \left[1 - \frac{(x-c.p)^{\alpha_{\text{right}}}}{(p-c.p)^{\alpha_{\text{right}}}} \right] & \text{when } c.p \leq x \leq p \end{cases} \quad (5)$$

This formula enables the exploration of a wide range of possible shapes. The symmetric triangular structure ($c=0.5$, $\alpha_{\text{left}}=\alpha_{\text{right}}=1$) and the asymmetric jagged scale structure ($c=1$, $\alpha_{\text{left}}=\alpha_{\text{right}}=1$) are only particular cases of this general expression. In total, six parameters can be varied.

4.1 Variation of p , h and $\varepsilon_{\text{form}}$

In the first optimization using the genetic algorithm, only three parameters of the structure were varied. The period $p=x_1$ ranged from $x_1^{\min}=1\mu\text{m}$ up to $x_1^{\max}=15\mu\text{m}$ by steps of $\Delta x_1=0.1\mu\text{m}$. The height $h=x_2$ was varied from $x_2^{\min}=1\mu\text{m}$ to $x_2^{\max}=10\mu\text{m}$ by steps of $\Delta x_2=0.1\mu\text{m}$. In this case, the height was cut off at $x_2^{\max}=10\mu\text{m}$ based on former results. The dielectric constant $\varepsilon_{\text{form}}=x_3$ of the material that constitutes the structure in itself was also varied from $x_3^{\min}=1.2$ to $x_3^{\max}=6.35$ by steps of $\Delta x_3=0.01$. $x_3^{\max}=6.35$ has been chosen as the highest considered value for the dielectric constant, as it is equal to the dielectric constant of the emitting material (GaN). The other parameters were fixed at $c=1$, $\alpha_{\text{left}}=1$ and $\alpha_{\text{right}}=1$.

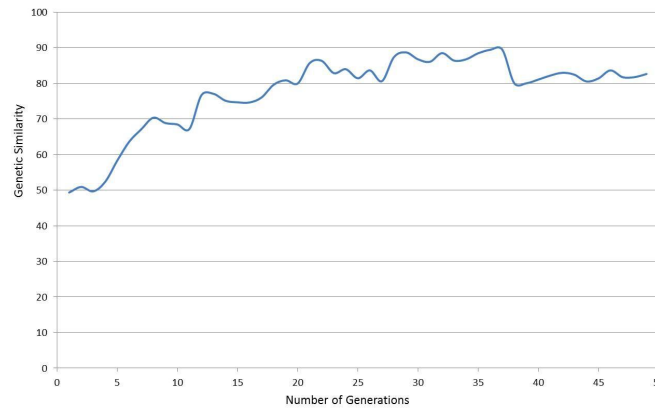


Figure 4. Genetic similarity for each generation when varying the period $p=x_1$, the height $h=x_2$ and the dielectric constant $\varepsilon_{\text{form}}=x_3$ of the structure.

Fig. 4 shows the evolution of the genetic similarity as a function of the number of generations. Generation after generation the genetic similarity increases. This increase is not steadily positive, as we introduce random seeds and mutation to explore a wider number of individuals in the parameter space. Therefore we encounter decreases in the genetic similarity.

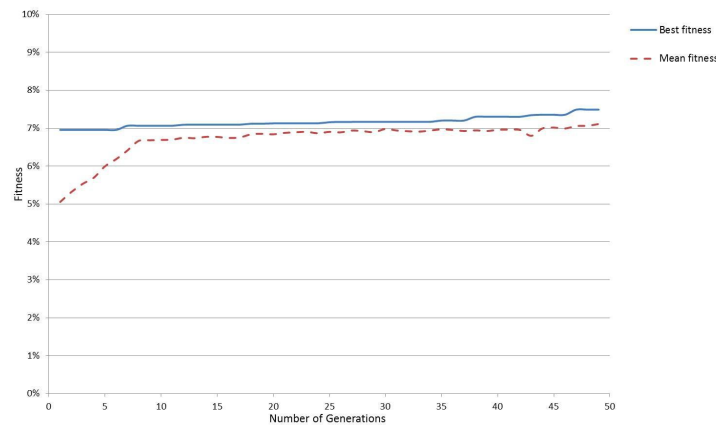


Figure 5. Fitness for each generation when varying the period $p=x_1$, the height $h=x_2$ and the dielectric constant $\varepsilon_{\text{form}}=x_3$ of the structure.

Fig. 5 shows the evolution of the fitness as a function of the number of generations. The genetic algorithm adjusts only three parameters in this case and the fitness converges very quickly to a high value. The mean fitness (dotted red line on Fig. 5) corresponds to the average fitness of all individuals of a given generation. For the first generation, one can see that the average fitness is close to the best value achieved by former, more gross, calculations. The best individual of the first generation is already significantly higher than the rest of the population. In this specific case, a solution providing a high fitness, i.e. a high LEE, is already achieved in the early stages of the optimization. The evolution of the genetic similarity shows however that the genetic algorithm

has still been exploring parameters and was therefore not stuck to a single high-fitness solution, thereby ruling out a local optimum.

In this simulation, the fitness reaches $\eta=7.5\%$ after 49 generations, which gives a relative increase in the LEE of $\Delta\eta=102\%$. This result corresponds to a period $p=x_1=2.98\mu\text{m}$, a height $h=x_2=2.20\mu\text{m}$ and a dielectric constant $\varepsilon_{\text{form}}=x_3=6.32$. It is interesting to note that a dielectric constant close to the value of the emitting material is more favorable for a high light-extraction efficiency. The structure determined by the genetic algorithm is represented in Fig. 6. This specific structure *doubles* the amount of light that is extracted in comparison to a plane surface.

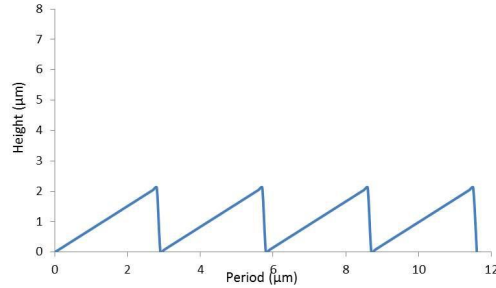


Figure 6. Profile of the structure associated with the highest LEE, as obtained for a period $p=x_1=2.98\mu\text{m}$, a height $h=x_2=2.20\mu\text{m}$ and a dielectric constant $\varepsilon_{\text{form}}=x_3=6.32$. The relative enhancement of the LEE reaches $\Delta\eta=102\%$.

The number of fitness evaluations in the present optimization reaches 1425, i.e. the light-extraction efficiency was calculated 1425 times. For the former results, 225 evaluations of the LEE were needed in order to determine an optimal shape for the jagged scale structure (see Sec. 2). Only two parameters were however considered (the period p and the height h) in this previous work, instead of three (p , h and the dielectric constant $\varepsilon_{\text{form}}$) in this optimization using the genetic algorithm. Moreover, the step width used with the genetic algorithm is way more precise than formerly. To achieve the same result by calculating all possible parameter combinations without using the genetic algorithm, over six millions evaluations would have been needed.

4.2 Variation of p , h , c , α_{left} and α_{right}

For this second optimization using the genetic algorithm, we considered the whole set of structural parameters (p , h , c , α_{left} and α_{right}). The dielectric constant of the material used for the surface texturation was fixed to a known, previously determined value ($\varepsilon_{\text{struct}} = 2.763$). Only the shape of the structure was thus changed. The period $p=x_1$ was varied between $x_1^{\text{min}}=1\mu\text{m}$ and $x_1^{\text{max}}=15\mu\text{m}$ by steps of $\Delta x_1=0.1\mu\text{m}$. The height $h=x_2$ was varied between $x_2^{\text{min}}=1\mu\text{m}$ and $x_2^{\text{max}}=10\mu\text{m}$ by steps of $\Delta x_2=0.1\mu\text{m}$. The height was cut off at $x_2^{\text{max}}=10\mu\text{m}$ just as in the previous case, based on former results. The apex position $c=x_3$ of the structure could take values between $x_3^{\text{min}}=0.5$ and $x_3^{\text{max}}=1$ by steps of $\Delta x_3=0.01$. This parameter controls the position of the apex. It allows the consideration of all intermediate structures between the symmetric triangle and the jagged scale structure (see Section 2). The concavity of the two edges can be changed independently, allowing the structure to have either convex or concave edges on any side. The concavity of the left edge is parameterized by $\alpha_{\text{left}}=x_4$, while the concavity of the right edge is parameterized by $\alpha_{\text{right}}=x_5$. These two parameters can take values between $x_{4,5}^{\text{min}}=0.2$ and $x_{4,5}^{\text{max}}=5$ by steps of $\Delta x_{4,5}=0.01$. $x_{4,5} \in [0.2, 1]$ corresponds to a convex edge. $x_{4,5} \in [1, 5]$ corresponds to a concave edge.

Fig 7 shows the evolution of the genetic similarity as a function of the number of generations. Fig 8 shows the evolution of the best and the mean fitness values as a function of the number of generations. Just as in the previous case (Sec. 4.1), the mean fitness value is comparable to the best LEE achieved when considering a systematic scan on parameters with larger discretization steps (see Sec. 2). However, already in the first generation, the best fitness indicates a significantly higher value for the LEE. This best fitness is increased further as more generations are considered. The genetic similarity is again an important indicator to verify a good exploration of parameters and that new individuals, very different from their parents, are taken into account to avoid local optima.

The highest LEE found by the genetic algorithm reaches $\eta=7.1\%$. This value is achieved for a period $p=x_1=6.87\mu\text{m}$, a height $h=x_2=4.97\mu\text{m}$, an apex position $c=x_3=0.51$, a concavity of the left edge $\alpha_{\text{left}}=x_4=1.07$

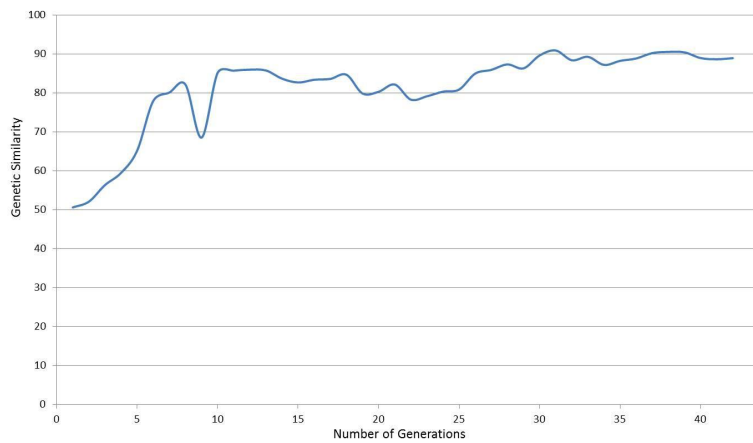


Figure 7. Genetic similarity for each generation when varying the period $p=x_1$, the height $h=x_2$, the apex position $c=x_3$ and the concavity of the edges $\alpha_{\text{left}}=x_4$ and $\alpha_{\text{right}}=x_5$.

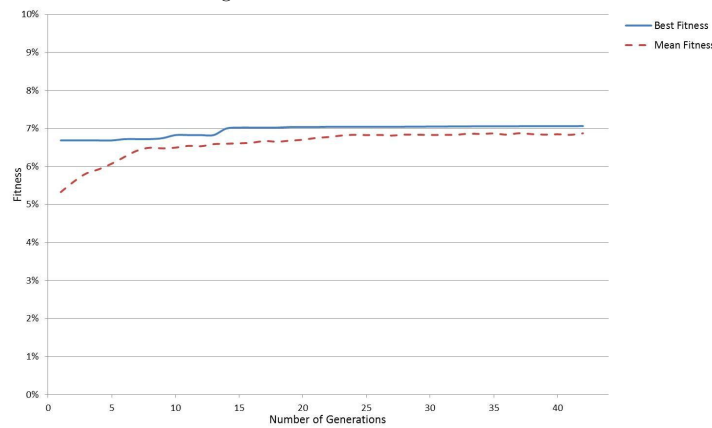


Figure 8. Fitness for each generation when varying the period $p=x_1$, the height $h=x_2$, the apex position $c=x_3$ and the concavity of the edges $\alpha_{\text{left}}=x_4$ and $\alpha_{\text{right}}=x_5$.

and a concavity of the right edge $\alpha_{\text{right}}=x_5=1.06$. The relative enhancement of the LEE reaches $\Delta\eta=89\%$. Fig. 9 represents the structure determined by the genetic algorithm.

The fitness function was calculated 1478 times to achieve the present result. In comparison to the results achieved in our previous work ($15 \times 15 \times 2=450$ evaluations for the jagged scale and the triangular shape, see Sec. 2) this might appear as a large number. However, we have to consider that in this case five parameters were varied instead of two, a wider variety of shapes was taken into account *and* the search was carried out with a higher precision than before. Only 1478 combinations out of 78 trillions were calculated.

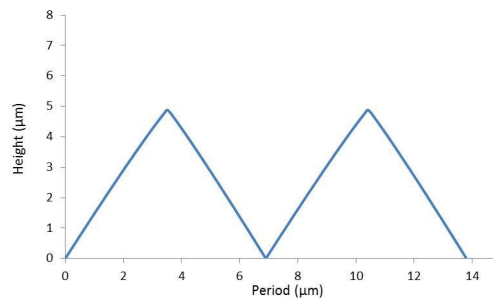


Figure 9. Profile of the structure associated with the highest LEE, as obtained for a period $p=x_1=6.87\mu\text{m}$, a height $h=x_2=4.97\mu\text{m}$, an apex position $c=x_3=0.51$, a concavity of the left edge $\alpha_{\text{left}}=x_4=1.07$ and a concavity of the right edge $\alpha_{\text{right}}=x_5=1.06$. The relative enhancement of the LEE reaches $\Delta\eta=89\%$.

5. CONCLUSION

We presented a method to increase the light-extraction efficiency of light-emitting diodes by using Nature as an inspiration. The first inspiration for the structures considered in this work came by studying thoroughly the morphology of a firefly. This structure was then studied in a wider approach by taking into consideration the specific needs of an artificial system, such as the light-emitting diode. The second inspiration from Nature that is used in this work is the genetic algorithm in itself, which mimics natural selection.

The results achieved with the genetic algorithm are more precise in the determination of structural parameters and also more accurate in the evaluation of the LEE than those achieved in our previous work, where every combination of parameters had to be considered. Here only a thorough selection is considered, which allows to take (a) more parameters into consideration and (b) a finer step width into consideration. The results found with the genetic algorithm are significantly higher than those achieved formerly.

When comparing the two optimizations presented in this paper, it is interesting to note that similar results could be achieved when working either on three or five parameters ($\eta \sim 7\%$). The first simulation introduced a variation of the dielectric constant $\varepsilon_{\text{form}}$, whereas the second simulation introduced a broader variation of the shape, taking into account the apex position c and the concavity of the two edges α_{left} and α_{right} . The optimization that included the dielectric constant could however provide higher light-extraction efficiencies. It seems that the dielectric constant of the add-on material has a very high impact on the final LEE.

The advantages of the genetic algorithm approach are obvious: we could explore a wider range of parameters, in a reasonable amount of time and achieve higher LEE. These simulations are still ongoing and even better results can be expected in the near future. A next step is to vary all six parameters to find an optimal structure for high light-extraction efficiency of LED's.

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