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# Hybrid genetic algorithm–tabu search approach for optimising multilayer optical coatings

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**Abstract**

Constructing multilayer optical coatings (MOCs) is a difficult large-scale optimisation problem due to the enormous size of the search space. In the present paper, a new approach for designing MOCs is presented using genetic algorithms (GAs) and tabu search (TS). In this approach, it is not necessary to specify how many layers will be present in a design, only a maximum needs to be defined. As it is generally recognised that the existence of specific repeating blocks is beneficial for a design, a specific GA representation of a design is used which promotes the occurrence of repeating blocks. Solutions found by GAs are improved by a new refinement method, based on TS, a global optimisation method which is loosely based on artificial intelligence. The improvements are demonstrated by creating a visible transmitting/infrared reflecting filter with a wide variety of materials.


*Keywords:* Optimisation; Genetic algorithms; Tabu search; Multilayer optical coatings

## 1. Introduction

Multilayer optical coatings (MOCs) are coatings which consists of a stack of thin layers of materials with differences in refractive indices [1]. Depending on the total number of layers, the composition and thickness of each layer, a MOC is able to reflect certain wavelengths while other wavelengths are transmitted unhindered [1]. This property allows the design of filters with specific spectral characteristics. An important use of MOCs is the use as a visible transmitting/infrared reflecting filter applied on halogen lamps. These types of filters increase the efficiency of halogen lamps by reflecting the infrared radiation, emitted by the filament, back to the filament for re-absorption and possible re-emission in the visible wavelength range. Energy losses due to energy being radiated in the infrared region are of the order of 80% for a halogen lamp operating at 2800 K but with the use of this type of filters, these losses can be reduced [2]. The synthesis of a visible transmitting/infrared reflecting filter has been the subject of a contest in 1996 [3].

Designing MOCs, or determining the optimal number of layers as well as the composition and thicknesses of each layer, is an elaborate optimisation problem, especially when considering that using state of the art deposition techniques, coatings can be made up of 75 or even more layers and a number of different materials can be used.

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Several methods are available for designing MOCs. They can roughly be divided into two categories: refinement methods and synthesis methods [4]. Refinement methods need a starting design which should be close to the optimal design, otherwise no good results are obtained. These methods usually modify the thicknesses of the layers but do not influence the total number or the sequence of the layers. Synthesis methods are more general. They create a promising design without a starting design. This promising design can be refined afterwards.

A recent development for designing MOCs is the introduction of genetic algorithms (GAs) [5]. The GA-based method can be classified as a synthesis method, as GAs do not require a starting design. By using GAs, a 90% rejection filter [5,6], a nonpolarising edge filter [7], an antireflection filter [6,7] and a beam splitter [6] were designed by Martin et al. [5–7]. These filters were designed for the wavelength range of 200 until 600 nm.

This paper introduces several improvements for designing MOCs with GAs, allowing for the design of more complex filters for a larger wavelength range. In this method, only the maximum number of layers is specified. The algorithm will decide how many layers are optimal. As it is generally recognised that the existence of specific repeating blocks can be beneficial for a design, a special GA representation of a design is used, which promotes the occurrence of repeating blocks. Solutions found by GAs are improved by a new refinement method, based on tabu search (TS), a global optimisation method which is loosely based on artificial intelligence. The improvements are demonstrated by creating a visible transmitting/infrared reflecting filter with various sets of materials. However, as this is a general system, it is possible to design a multitude of different MOCs.

## 2. Theory

### 2.1. Genetic algorithms

GAs are a special class of global optimisers, based on the theory of evolution. A GA is able to minimise (or maximise) a function $G(x)$, where $x$ represents a parameter vector, by searching the parameter space of $x$ for the optimal solution [8,9]. GAs do not operate on a single trial solution, but on a group of solutions, called a population. A solution, which is called a string, is a vector of all parameters which are to be optimised. Using evolutionary inspired operators such as fitness, crossover and mutation, the best solutions are modified and passed on to the next generation. In this way, the population as a whole moves towards better solutions, ideally to the global optimum. For a better understanding of GAs the reader is referred to [9,10].

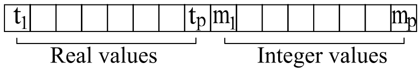


Fig. 1. Example of the representation of a design with a maximum of eight layers in GAs. The representation is a mixture of real values for the thicknesses ($t$) and integer values for the material types ($m$).

#### 2.1.1. Representation

A trial solution, containing values of all parameters that are to be optimised, can be represented by a vector of bits, real values or integers. A design consisting of $p$ layers is completely described by a vector, one half containing the thicknesses of each layer $t = t_1, \ldots, t_p$ and one half containing the type of material per layer $m = m_1, \ldots, m_p$. Therefore, the search space for designing MOCs consists of real values for the thicknesses and integer values indicating what type of material is used for each layer. Fig. 1 shows a schematic of the representation used in the GA. This is also the representation used in the work of Martin et al. [5–7]. In addition, a few improvements are introduced. If a solution is to be found with three types of material, these types are indicated by 1, 2 and 3. The first major improvement is the introduction of a zero-type material in the representation. When the material type is zero, a layer will have no material assigned to it and it will not be used in the design. In this way, the number of layers in a design is flexible, and the GA can decide how many layers actually will be present in a design. Only the maximum number of layers has to be specified. After applying the GA operators to a string, a cleanup and back coding of this string is performed. This is a consequence of using the zero-type material. An example of the cleanup process and the back coding is shown in Fig. 2. Two adjacent layers with identical material types are combined into one thicker layer and layers with a zero material type are removed.

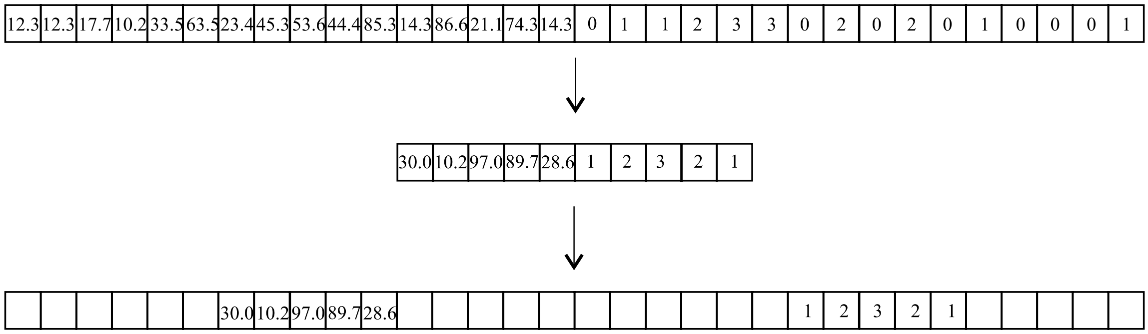


Fig. 2. Example of the cleanup process of a string and of putting the cleaned up design back to the string. A random offset (in the example six is used) determines the position were the design is put back. Empty places in the lower string are filled with zeros, but these are omitted for clarity.

After this cleanup, each design is coded back to the GA string. A further essential improvement is that the representation for a design is not coded back starting at position zero in the GA string, but at a random position. In this way, the representation of a design can move across the complete string in the GA and is not only located at the first part of a string. When applying the crossover operator during a GA run, it is now possible to copy complete blocks from one string to another. After applying a number of crossover operators, it is possible that, within one string, a block is repeated. The repeated occurrence of specific blocks is considered beneficial for the performance of a design. Layers in the beginning or end in the GA representation which are not used, are given a zero material type. At the beginning of a GA run, the first generation is seeded with small designs. These design have only a few layers with a material index other than zero. Positions in a string which are not used are given material type zero.

#### 2.1.2. Evaluation function

The quality of a solution is given by the fitness value, which is calculated by the evaluation function. The fitness value is used by the GA to discriminate between good and not so good designs, so it can select accordingly. For optical filters, the fitness of a design is determined by calculating the corresponding transmission spectrum using the matrix formalism [1,11]. This spectrum is compared with a target transmission spectrum by using evaluation function $F$, which sums the differences between the intensities of the calculated transmission spectrum, indicated by $T(\lambda)$, and the target transmission spectrum, indicated by $\tau(\lambda)$, as shown in Eq. (1):

$$F = \sum_{\lambda=\lambda_{\min}}^{\lambda=\lambda_{\max}} \frac{|\tau(\lambda) - T(\lambda)| \cdot W(\lambda)}{N} \tag{1}$$

The differences in intensities are multiplied by a weighting factor $W(\lambda)$ to stress the relative importance of some areas over others. $N$ indicates the number of wavelengths in the transmission spectrum. The resulting evaluation value $F$ is minimised by the GA. By changing the target transmission spectrum $\tau(\lambda)$ it is possible to construct filters with specific properties. The target spectrum, in combination with a set of weights, determines what kind of filter is designed. Fig. 3 gives a few examples of target spectra, corresponding to a beam splitter, a visible reflecting/IR transmitting and a 90% rejection filter.

### 2.2. Refinement with tabu search

GAs are able to locate promising regions for global optima in a search space, but sometimes have difficulty finding the exact minimum of these optima [9]. Especially, since the search space for constructing a visible transmitting/infrared reflecting filter is very large, it is likely that designs found by GAs can still be improved. Several examples are known from literature where a solution, obtained by GAs, are improved by a second optimisation method [12–14]. In this paper, a new procedure, based on TS, is used to refine the designs. Where GAs are inspired by the process of evo-

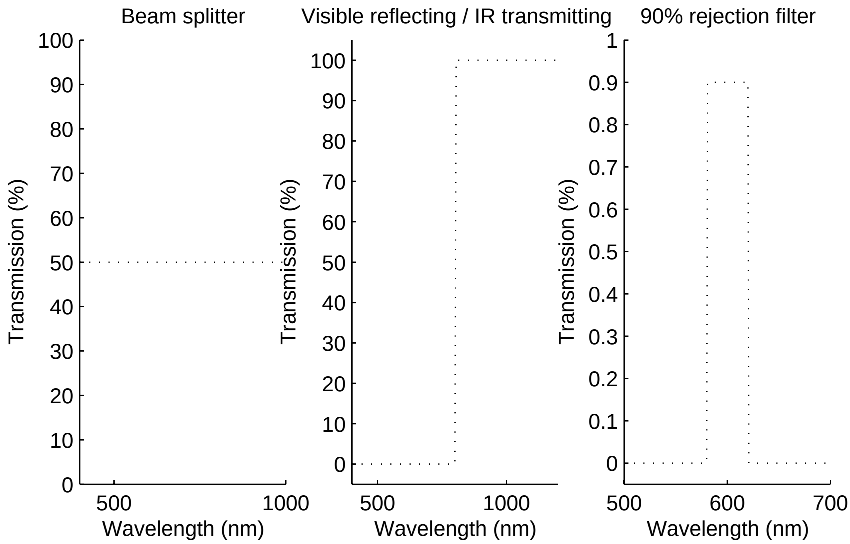


Fig. 3. Examples of different target spectra for the construction of filters with different characteristics. The target spectrum for a beam splitter (left), a visible reflecting/IR transmitting filter (middle), a 90% rejection band filter (right).

lution and work on a group of solutions at a time, TS is based on concepts from artificial intelligence and operates on a single solution at a time [15]. TS uses basic, problem-specific operators to explore a search space and memory (which is called the tabu list) to keep track of parts already visited. By guiding the optimisation to new areas, TS is able to overcome local minima and hopefully reach the global optimum. Refining MOCs with local optimisers could easily yield poor results, since the search space is very complex and consists of many local optima in which a local optimisers would get stuck. The foundations for TS were laid out in the late 1970s by Glover and the principles were described in general terms in 1989 and 1990 by Glover [16–18]. In recent years, tutorials documenting successes accomplished with TS have been published [15,18,19]. The framework of TS consists of several steps which are described below and depicted in Fig. 4.

(1) *Initialisation*: A starting design $s$ is chosen. For the construction of simple filters, this starting design can be chosen randomly. Here, the best result from the GA is used.
(2) *Neighbourhood exploration*: All possible neighbours of design $s$ are generated and evaluated. A neighbour is a design which can be reached from the current design by a simple, basic transformation of this current design. Two neighbouring designs resemble each other closely. For refinement of MOCs, the sequence of materials will be kept as it resulted from the GA run and only the thicknesses of the layers will be adjusted. Each thickness in turn can be adjusted by adding or subtracting a small random value. So, during one iteration, $2p$ neighbours have to be evaluated for a design with $p$ layers.

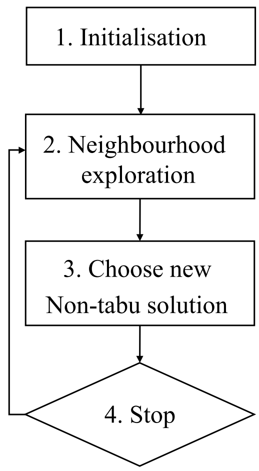


Fig. 4. General flowchart of the tabu search algorithm.

(3) *Choose a new nontabu design*: A new design is chosen from the explored neighbourhood. This design has the best fitness value from all neighbours and is not in the tabu list. The tabu list keeps track of previously explored designs and prohibits TS from revisiting them again. Thus, if the best neighbouring design is worse than the current design, TS will go uphill. In this way, local minima can be overcome. Instead of storing previously explored designs, it is also possible to store moves (changes to previous designs). Any reversal of these moves is then tabu, and they will remain so for a prespecified number of iterations.
(4) *Stop*: If no more neighbours are present (all are tabu), or when during a predetermined number of iterations no improvements are found, the algorithm stops. Otherwise, the algorithm continues with step (2).

## 3. Experimental

The left part of Fig. 5 shows the target requirements for a visible transmitting/infrared reflecting filter, viz. 100% transmission in the visible wavelength range and zero transmission in the infrared region. In the evaluation function, a weight of 5.0 is given to the visible wavelength range, as it is important that the transmission is as high as possible. For the infrared range, the weights are determined differently because the spectral power distribution of a tungsten coil is not constant in the IR range [2]. To emphasise areas which have more output, the wavelengths in the IR range are weighted with the coefficients of a black body radiator at 3000 K. All weights are shown in the right part of Fig. 5. Transmission spectra were calculated from 380 to 2000 nm with a total of 200 datapoints. The sampling rate for calculating the transmission spectra was 5 nm in the visible wavelength range and 10 nm in the infrared range.

Several visible transmitting/infrared reflecting filters were constructed using four different combinations of materials. A combination consists of a material with a low refractive index ($SiO_2$, for instance) and a high refractive index (rutile $TiO_2$ or SiC, for instance). The choice of materials greatly influences the quality of the filters after optimisation. To demonstrate the influence of the number and the properties of the materials and the ability of the GA–TS approach, several combinations of materials are tested. The combinations are shown in Table 1 and described as follows:

(1) Combination I consists of $SiO_2$ and $Nb_2O_5$. These materials are currently in use for sputtering visible transmitting/infrared reflecting filters.

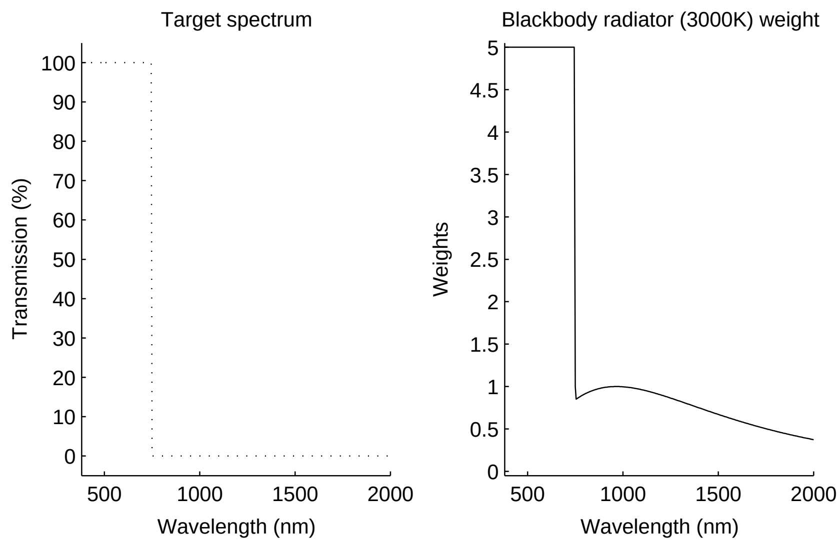


Fig. 5. Target spectrum (left) and weights (right) for the visible transmitting/infrared reflecting filter problem.

Table 1
The materials used in each combination with refractive indices at 550 nm

| Combination | $n_{low}$ | $n_{intmed}$ | $n_{high}$ | Properties |
|---|---|---|---|---|
| I | $SiO_2$ 1.46 | – | $Nb_2O_5$ 2.34 | Dispersive/absorbing |
| II | $SiO_2$ 1.46 | $ZrO_2$ 2.06 | Rutile $TiO_2$ 2.74 | Dispersive/absorbing |
| III | $SiO_2$ 1.46 | $ZrO_2$ 2.06 | Rutile $TiO_2$ 2.74 | Dispersive/nonabsorbing |
| IV | $MgF_2$ 1.35 | $ZrO_2$ 2.00 | SiC 2.60 | Nondispersive/nonabsorbing |

(2) Combination II consists of $SiO_2$, $ZrO_2$, and rutile $TiO_2$. Currently, filters are used which are based on two materials (as in combination I). However, in the future, filters based on three different materials will be used, as it is expected that with three different materials more efficient filters can be constructed [11]. The combination of materials is chosen in such a way that the refractive indices are ideal for a three material system. As a rule of thumb, when the refractive index of the intermediate material equals the square root of the product of the refractive indices of the other two materials, the refractive indices are considered optimal [11]. Both the dispersive and absorbing properties of the materials in combinations I and II have been taken into account, which is closest to reality.

(3) The materials in combination III are identical to combination II. However, in this combination, nonabsorbing properties have been assumed for all materials. Assuming nonabsorbing properties, is forcing the materials to behave more ideally. This should have a positive effect on the resulting filter and demonstrates the negative influence of the absorptive properties and thus the need for nonabsorbing materials.

(4) Combination IV consists of $MgF_2$, $ZrO_2$ and SiC. Again, this is a three material system which is expected to perform very well. It represents the case were the properties of materials are ideal (nondispersive and nonabsorbing). In this case, the materials also span a wide range of refractive indices. Using materials which span a wide range in refractive indices is considered beneficial for the construction of a visible transmitting/infrared reflecting filter [2]. The refractive index of the intermediate material ($ZrO_2$) has, just as in combinations II and III, the ideal value in combination with $MgF_2$ and SiC.

The wavelength dependencies of the refractive indices for the materials are shown in Fig. 6. For all combinations, the incident medium was air, normal incidence was assumed and glass was used as a substrate.

The optimal search settings of the GA and TS were determined based on previous experience and by trial and error. The settings are shown in Tables 2 and 3. The maximum number of layers was set to 60. The initial population was seeded with designs which contained a maximum of six layers, with thicknesses ranging from 10 to 75 nm. During a run, the lower limit for the thickness of a layer was set to 10 nm, while there was no upper limit.

All software was programmed in ANSI-C. GA calculations were performed using the GA library PGAPack, version 1.0 [20]. TS was programmed from

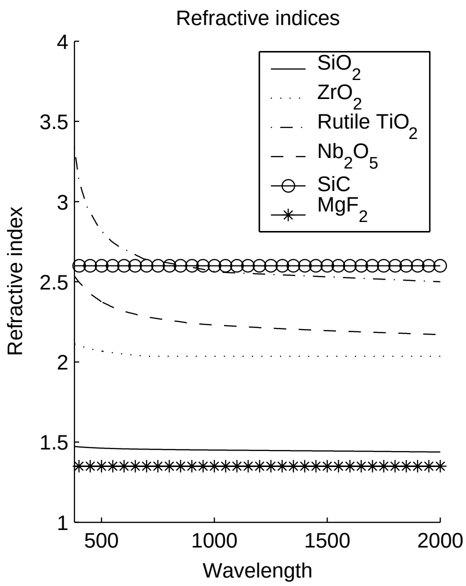


Fig. 6. Refractive indices for the material types.

Table 2
Settings used for GA optimisation

| Setting | Value |
|---|---|
| Number of generations | 250 |
| Population size | 600 |
| Elitism | 50 |
| Crossover type | Two-point |
| Crossover probability | 0.7 |
| Mutation type | Gaussian distribution with zero mean and standard deviation of 0.4 |
| Mutation probability | 0.05 |
| Selection type | Tournament selection |
| Fitness type | Raw |

Table 3
Settings used in the TS-refinement of layer thicknesses in GA-generated designs

| Setting | Value |
|---|---|
| Stepsize | Random value within 0–5 nm |
| Length of tabu list | 20 iterations |
| Number of iterations without improvement | 50 |

scratch. Calculations were performed on a Sun-Ultra 10 running at 440 MHz. Runtimes were in the order of 15 min per run. The GA runs were repeated with different random seeds to exclude any negative effects of the random starting population. At the end of a GA run, only designs which have a transmission average of over 96.5% in the visible range are considered. An average below 96.5% is considered too low to yield an effective filter.

## 4. Results and discussion

The left parts of Figs. 7–10 show the best transmission spectra after applying the GA method and refinement with TS when using the combinations of materials from Table 1. In each of these figures, the dashed line indicates the target spectrum. Table 4 contains the characteristics of all four spectra. In Fig. 7, the dotted line indicates a transmission spectrum of a filter which is currently used on halogen lamps. This reference design uses the materials of combination I,

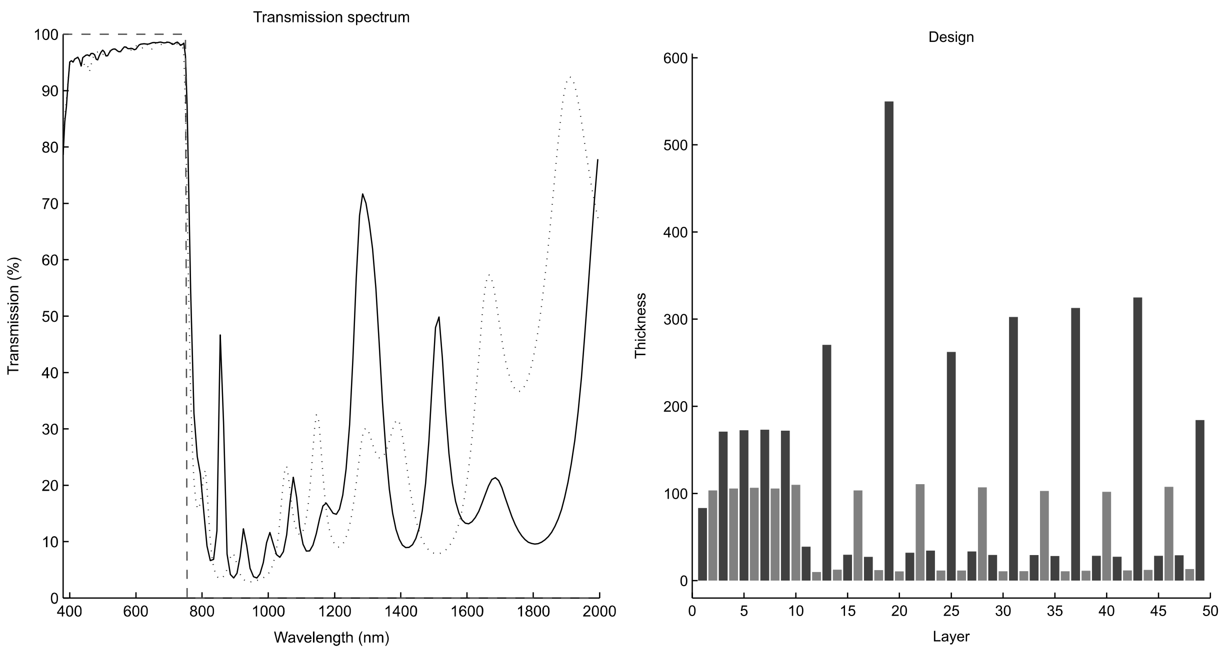


Fig. 7. Transmission spectrum (left, solid line) and the thicknesses for each layer (right) for the design with combination I. The target spectrum is shown with the dashed line, the dotted line is the transmission spectrum of a reference filter which is actually used on halogen lamps (left). Black indicates $SiO_2$, grey indicates $Nb_2O_5$ (right).

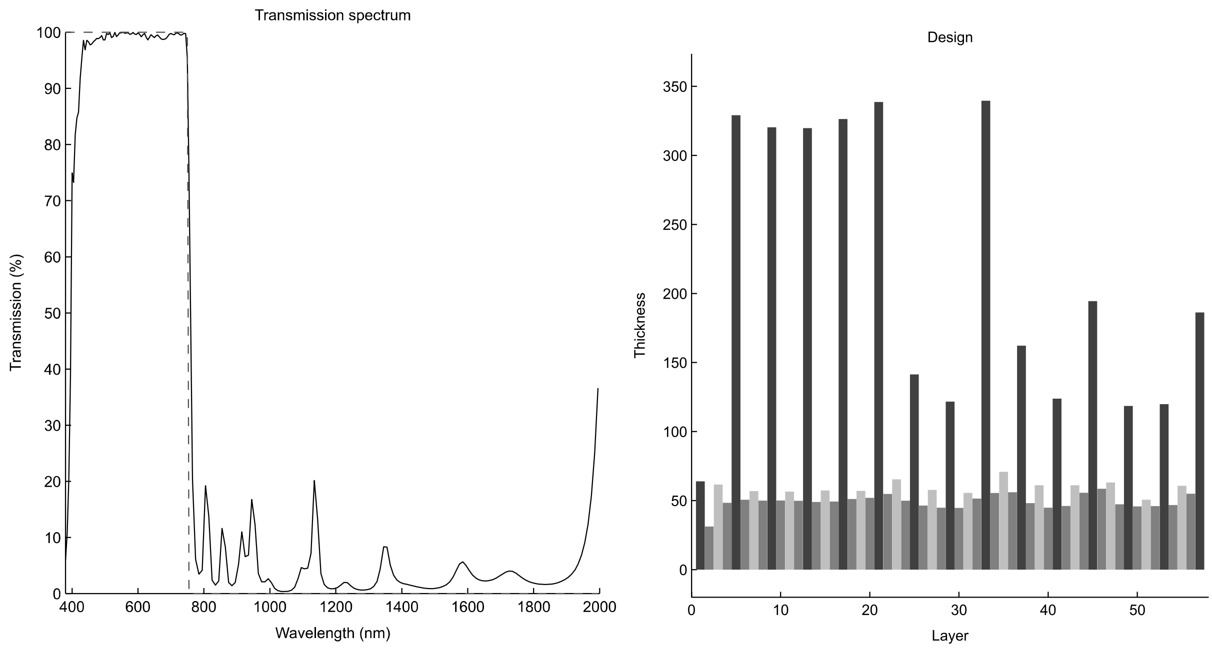


Fig. 8. Transmission spectrum (left, solid line) and the thicknesses for each layer (right) for the design with combination II. The target spectrum is shown with the dashed line (left). Black indicates $SiO_2$, dark grey indicates $ZrO_2$, light grey indicates rutile $TiO_2$ (right).

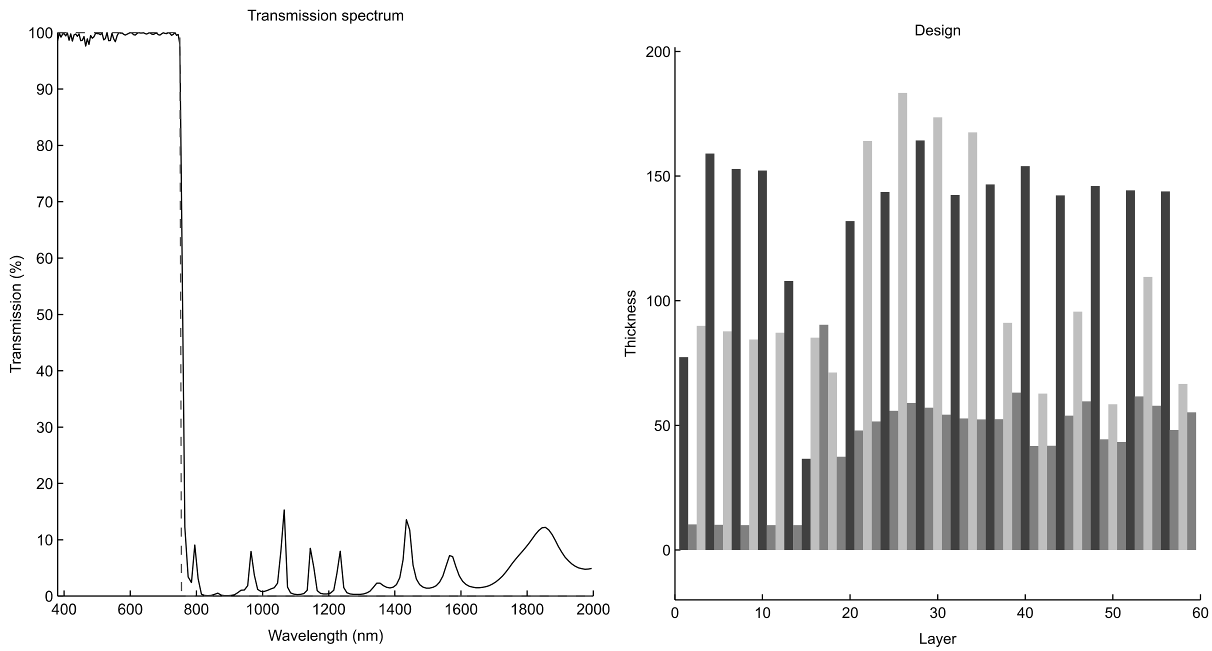


Fig. 9. Transmission spectrum (left, solid line) and the thicknesses for each layer (right) for the design with combination III. The target spectrum is shown with the dashed line (left). Black indicates $SiO_2$, dark grey indicates $ZrO_2$, light grey rutile $TiO_2$ (right).

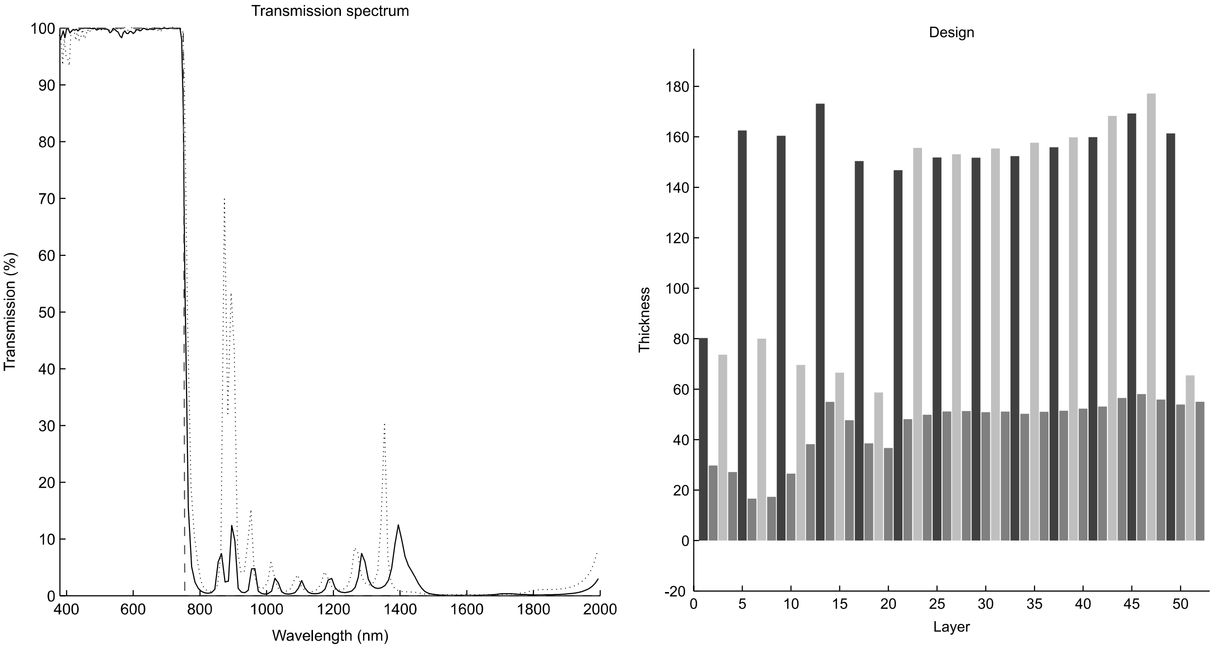


Fig. 10. Transmission spectrum (left, solid line) and the thicknesses for each layer (right) for the design with combination IV. The target spectrum is shown with the dashed line, the dotted line indicates the transmission spectrum after the GA-run but before the TS refinement (left). Black indicates $MgF_2$, dark grey indicates $ZrO_2$, light grey indicates SiC (right).

consists of 47 layers and was created by refinement of a stack of blocks which influence different spectral ranges. The number of layers was kept constant during the design of this reference filter. The design located with GAs transmits an equal amount of radiation in the visible region but is able to reflect 7% more radiation in the IR range. The right parts of Figs. 7–10 show the composition of each design together with the thicknesses per layer in nm. All GA-runs start with completely random designs of only a few layers, but in the end, the best designs show a high degree of repetition, like one would expect when using analytical methods for filter design. Apparently, the GA–TS approach mimics the results of analytical methods.

When comparing the transmission spectra obtained with combinations I and II, the results are better for combination II which has three materials. The reflective properties for combination II in the IR range are good. However, mainly due to the absorbance of rutile $TiO_2$ in the visible wavelength range, wavelengths near 400 nm are absorbed by the filter, as shown in Fig. 8. A lamp coated with a filter based on this design will not be colour neutral and will have limited applicability. Restricting the use of rutile $TiO_2$ improved the

Table 4
Average transmittances for the visible and IR wavelength range for each combination of materials from Table 1, together with the number of layers, physical thickness and measure of improvement for refinement with TS and the number of TS iterations

| Combination | Visible | IR | Layers | Thickness (nm) | TS improvement (%) | TS iterations |
|---|---|---|---|---|---|---|
| I | 96.6 | 22.1 | 49 | 4690 | 11 | 277 |
| Reference MOC Fig. 7 | 96.5 | 29.4 | 47 | 3718 | – | – |
| II | 93.5 | 4.8 | 57 | 5421 | 22 | 409 |
| III | 99.5 | 4.2 | 59 | 5056 | 52 | 375 |
| IV | 99.4 | 2.2 | 52 | 4690 | 56 | 754 |

performance in the visible wavelength range, but deteriorated the performance of the IR wavelength range considerably. In combination III, nonabsorbtivity of all materials has been assumed. Immediately, results increased in quality, as the best transmission spectrum, shown in Fig. 9, greatly improves.

The best results are obtained with combination IV in Table 1, where both materials have nondispersive and nonabsorbing properties. In this example, transmission averages in both the visible and IR wavelength ranges have excellent properties. When using nondispersive and nonabsorbing materials for filter design, the problem is somewhat simplified which leads to a simpler search space and, subsequently, to the location of better solutions.

The use of more than three materials yielded no better designs. As the GA is capable of selecting the materials, it often used mainly three materials when four materials were offered. It seems more important that the three materials span a reasonable range of refractive indices.

The number of layers is not constant during a GA run. Fig. 11 shows the number of layers in the best design of each generation for combination II from Table 1. In the beginning of a run, the best designs contains a very small number of layers and during a run, this number steadily increases. It is very likely that the best solution will contain a large number of layers (but still below the maximum) since better designs can be created with more layers [11].

Refinement with TS is a worthwhile process as all designs optimised with GAs could still be improved by TS. GAs are able to locate promising designs, but lack a certain precision to obtain the exact (global or local)

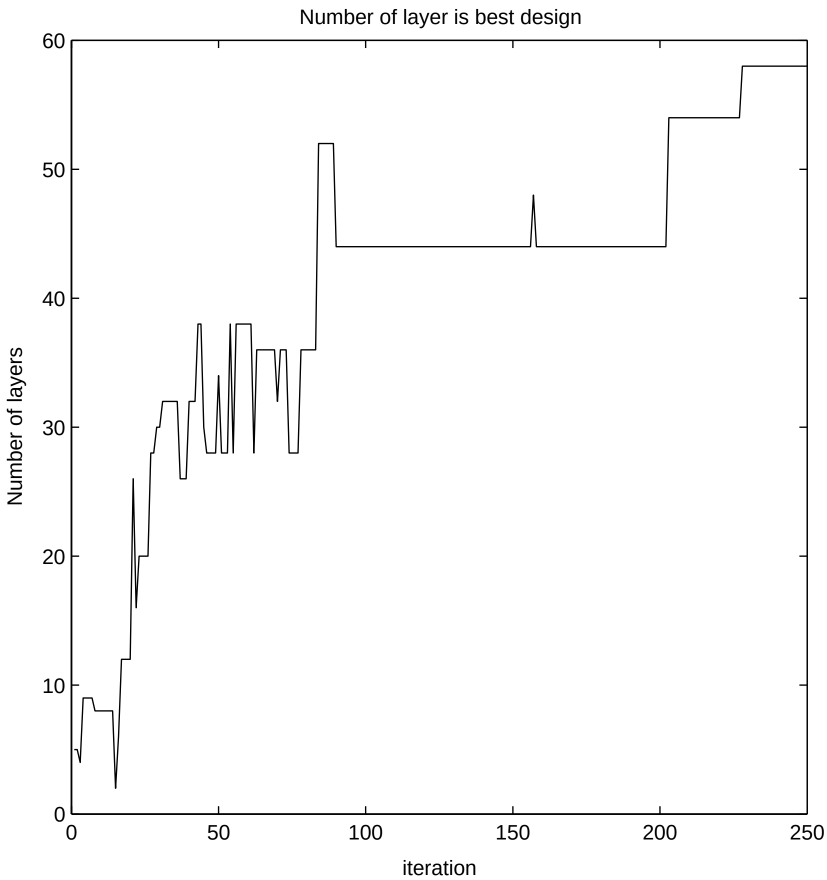


Fig. 11. The number of layers in the best design in each iteration.

minimum. This minimum is obtained by refinement with TS.

The improvements in evaluation value $F$ for all four combinations are shown in Table 4 and range from 11 to 56%. The main improvements in the transmission spectra for all four combinations are located in the IR range. The visible range usually performs well after the GA optimisation. The largest improvement (56%) can be found for combination IV. In the left part of Fig. 10, the best design obtained with the GA is shown with the dotted line. After refinement with TS (shown with the solid line), the transmission spectrum clearly shows improvement, mainly reached by the decrease of the large transmission peak around 900 nm. The number of iterations for the TS refinement varies somehow, the minimum being 277 (combination I), the maximum being 754 iterations (combination IV).

In this approach, TS is used for refining designs which were obtained with GAs. However, designing simple filters without a good starting point is also possible with TS. When using two materials, an alternating sequence of materials is used. When using more than two materials, the sequence of materials also needs to be optimised. If the sequence has to be optimised with TS, it is necessary to determine operators which modify the material type of a layer when a neighbourhood is explored. However, in the approach demonstrated here, it is shown that GAs are very well able to establish a good sequence of materials with reasonable values for the thicknesses. These thicknesses can be refined with TS with good results.

It is unknown how the filters, optimised in this paper, will perform when implemented. Since small errors in the deposition of layers could change the characteristics, some changes could be expected. It is possible to create filters which are more robust against small deviations in thicknesses. To asses the influence of these deviations, filters can be evaluated multiple times while some random deviations to the thicknesses of the layers have been added. Filters which are sensitive to these deviations while deteriorate more and get a lower evaluation value. In the end, the obtained filter will be more robust.

It is also possible to perform the TS refinement during a GA run and refine the members of the GA population at each generation. It might be possible, due to synergetic effects, that better solutions might be obtained. However, calculation times would become too long and this makes any practical application virtually impossible.

The transmission spectra obtained with the GA–TS method for constructing a visible transmitting/IR reflecting filter, cannot directly be compared with results from the contest [3]. The contest used different materials, a different evaluation function which also took into account the number of layers while the wavelength ranges between 380–400 and 720–750 were left out. However, these wavelengths are crucial for some real-world applications, such as the halogen lamp filters. Furthermore, it was not necessary to penalise larger designs compared to smaller designs because in our approach only a maximum number of layers was important.

## 5. Conclusion

As a typical design for a MOC can contain up to 75 layers, each with their own thickness and material type, the search space for creating MOCs is enormous, which makes constructing MOCs a difficult optimisation process.

In this paper, several improvements are introduced for optimising MOCs with GAs. Firstly, the representation employed, including a zero-type material, makes it unnecessary to specify beforehand how many layers will be present in a design. The algorithm can decide this, which is very efficient. Secondly, the special cleanup of the GA representation of a MOC and subsequently back coding at a random position makes it possible, by applying the crossover operator, to copy complete blocks from one design to another design at any position. The repeated occurrence of blocks is considered beneficial for the performance of MOCs. Finally, GAs are able to locate promising designs, but lack a certain precision. Designs optimised with GAs, are refined by a new refinement method, based on TS. TS refinement leads to improvements in the range of 10–50% for the examples shown in this paper.

All the improvements are demonstrated by the creation of a visible transmitting/infrared reflecting filter using several combinations of materials. The choice and number of materials influences the quality of the best designs. As expected, the use of three materials yielded better designs compared to the use of two materials. Using dispersive and absorbing materials make it harder to obtain a good filter, for instance in combination II where the specific absorbance of rutile $TiO_2$ is a problem. Using nondispersive and nonabsorbing materials yield good filters by simplifying the problem. This also stresses the importance of the use of materials with the correct properties. Three materials, with no or a minimum of absorbing or dispersive properties and a large difference between the lowest and highest refractive index, while the third has an intermediate value, seems to work the best. As this is a very general method, it is possible to design a multitude of different MOCs.

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