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A multi-objective genetic algorithm for the optimization of a solar thermal collector

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Abstract: We present a multi-objective genetic algorithm we developed for the optimization of a solar thermal collector. This collector consists of a waffle-shaped Al substrate with NiCrO$_x$ cermet and SnO$_2$ anti-reflection conformal coatings. Optimal geometrical parameters are determined in order to (i) maximize the solar absorptance $\alpha$ and (ii) minimize the thermal emittance $\varepsilon$. The multi-objective genetic algorithm eventually provides a whole set of Pareto-optimal solutions for the optimization of $\alpha$ and $\varepsilon$, which turn out to be competitive with record values found in the literature. In particular, a solution that enables $\alpha = 97.8\%$ and $\varepsilon = 4.8\%$ was found.

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References and links

1. Introduction
Solar thermal collectors are a nice example of the use of a renewable energy, i.e. the Sun, since without the need of additional electric energy consumption they allow to heat water for domestic use or even for producing electricity from collected thermal energy.[1, 2] Amongst all possibilities for producing solar absorbers,[3] cermets, in the form of thin films, are today the only industrial alternative. Cermets are nanostructured composites in which metallic nanoparticles are embedded in a ceramic matrix. This structure is especially adapted for strong absorption in the UV-visible region, due to plasmonic absorption in the particles and interband electronic transitions in the matrix.[4] As the cermet coating is deposited on an IR-reflective substrate, its IR-transparency actually allows the solar collector to have a low emittance, therefore reducing thermal losses. Many cermet materials such as Ni-Al$_2$O$_3$, Cr-Cr$_2$O$_3$, Al-AlN and Ni-NiO are known to be good candidates.[5, 6, 7, 8] Thanks to a previous work by Gaouyat et al.,[9, 10] Ni-NiCrO$_x$ was found to be an ideal candidate for solar absorber applications because of its various absorption mechanisms. In order to reach higher performances, cermets are always coupled with an anti-reflection layer in a tandem absorber system.[11] Tin oxide was chosen for its ability to be produced by sputtering in addition to its anti-reflective property. It was proven in a previous work that a structuration of the substrate can lead to a further increase of the absorption.[12] Following the study of Shimizu et al.,[13] we will consider waffle-like patterns consisting of the periodic repetition of truncated inverted pyramids. The confrontation of tandem solar absorbers with and without substrate structuration will be considered in this study in order to understand the role of this additional feature.

The optothermal properties of solar absorbers are characterized by two quantities: the solar absorptance $\alpha$ and the thermal emittance $\varepsilon$. They describe respectively the absorber ability to harvest the sun radiation and to avoid thermal losses calculated from the black-body spectrum of the absorber. In order to maximize the efficiency of the collector, the solar absorptance $\alpha$ should be maximized and the thermal emittance $\varepsilon$ should be minimized. We hence need to conjointly optimize $\alpha$ and $\varepsilon$ in order to achieve an efficient collector. This optimization is often done empirically since a complete investigation of all possible combinations of parameters would be untractable. The usual parameters are the thicknesses of the layers or the metal content of cermet layers.[11] In the present work, the parameters to be optimized are not only the thicknesses of the tandem absorber layers (NiCrO$_x$ and SnO$_2$), but also the geometrical parameters...
depends on the parameters \( x \) the representation of each parameter. We want to find, amongst this whole set of possibilities for \( \{ x \} \), representatives of a given set of parameters. Every developer of a genetic algorithm will finally implement his own tricks to converge more efficiently to the solution. For a given implementation of a genetic algorithm, a decision must be taken for the size of the population, the rate of crossover and the rate of mutation. This is essentially done from experience.

We present in this work a multi-objective genetic algorithm we developed for the optimization of a solar thermal collector that consists of a waffle-shaped Al substrate with NiCrO conformal coatings. The geometrical parameters of this system must be adjusted in order to achieve two objectives: (i) to maximize the absorptance \( \alpha \) and (ii) to minimize the emittance \( \varepsilon \). The details of this algorithm are presented in Sec. II. Sec. III then presents the results achieved with the solar thermal collector. Sec. IV finally concludes this work.

2. Multi-objective genetic algorithm

Let \( f = f(\vec{x}) \) be an objective function of \( m \) components \( f_j(\vec{x}), \ldots, f_m(\vec{x}) \). Each component \( f_j(\vec{x}) \) depends on \( n \) physical parameters \( x_i \), where \( x_i \in [x_i^{\text{min}}, x_i^{\text{max}}] \) with a specified granularity of \( \Delta x_i \) in the representation of each parameter. We want to find, amongst this whole set of possibilities for the parameters \( x_i \), the values that maximize globally the different components of the objective function.

Each parameter \( x_i \) is actually represented by a string of \( n_i \) bits (0 or 1), also called a "gene". \( n_i \) is chosen so that \( (x_i^{\text{max}} - x_i^{\text{min}})/(2^{n_i} - 1) \leq \Delta x_i \). The value of the physical parameter \( x_i \) is then given by \( x_i = x_i^{\text{min}} + (\text{gene } i) \times \Delta x_i \), where \( (\text{gene } i) \in [0, 2^{n_i} - 1] \) stands for the value coded by the gene \( i \) in Gray binary coding. The genetic algorithm must reject gene values that lead to \( x_i > x_i^{\text{max}} \) in order to achieve a strict enforcement of our parameter specifications. A given set of parameters \( \{ x_i \} \) is finally represented by the juxtaposition of the \( n \) genes used for the representation of each parameter. These strings of \( n \) genes are also called "DNA". The genetic algorithm actually works on the DNA representation of parameters when searching for optimal solutions.

We work with a population of \( n_{\text{pop}} = 100 \) individuals. Each individual has its own DNA. It is therefore representative of a given set of parameters \( \{ x_i \} \). The initial population usually consists of random individuals. These individuals must be evaluated in order to determine the corresponding values of the objective function \( f \). We must also define an effective fitness function \( f_{\text{eff}} \) for the classification of these individuals. Working with \( f_{\text{eff}} = \sum_{j=1}^m w_j f_j \), where \( w_j \) are arbitrary weighting factors, would lead the GA to optimize a specific linear combination of the components \( f_j \) of the objective function, without taking into account how individuals actually compare for each \( f_j \). We will work instead with an effective fitness function \( f_{\text{eff}} \) that depends on the Pareto-classification of these individuals. This classification is based on the concept of dominance: a solution \( \vec{x}_1 \) is dominated by the solution \( \vec{x}_2 \) if \( f_j(\vec{x}_2) \geq f_j(\vec{x}_1) \forall j \) and \( \exists j : f_j(\vec{x}_2) > f_j(\vec{x}_1) \). Pareto-optimal solutions are solutions that are not dominated. The effec-
tive fitness $f_{\text{eff}}$, which is given with details in the Appendix, will be higher for individuals that are not dominated. This will force the GA to establish a whole set of Pareto-optimal solutions, instead of just focussing on a specific linear combination of the $f_j$.

The individuals are then sorted according to this effective fitness. $n_{\text{pop}}/2$ individuals ("the parents") are selected by a rank-based "Roulette Wheel Selection".[17, 18] This is a random selection procedure in which the probability for an individual to be selected is proportional to its weight on a "wheel". The individual with the highest effective fitness receives a weight equal to $n_{\text{pop}}$, the second-best individual receives a weight equal to $n_{\text{pop}} - 1$, etc. The last individual receives a weight equal to 1. Individuals with a higher effective fitness have thus more chance to be selected. A given individual can be selected several times. This enables the best individuals to progressively dominate the population.

The parents are transferred to the next generation. In addition, they generate new individuals ("the children"). For any pair of parents, two children are obtained either (i) by a one-point crossover of the parents’ DNA (probability of 90%), or (ii) by a simple replication of the parents’ DNA (probability of 10%). The position in the chain of bits at which the two parts of the parents’ DNA is exchanged is chosen randomly.[17, 18] The transmission of unchanged individuals to the next generation enables the conservation of good solutions. The exploration of new solutions is achieved by the individuals obtained when crossing the parents’ DNA. We finally introduce random mutations: each bit of the children’s DNA has a probability of 1% to be reversed. This is an essential ingredient for the exploration of parameters. It enables indeed a final refinement of the parameters.

These steps of selection, crossover and mutation must be repeated from generation to generation until convergence is achieved (maximum of 100 generations). By this game of natural selection, the genetic algorithm will progressively determine optimal solutions for the problem considered. We implemented elitism in order to make sure that the individuals that provide the best values for $f_1, \ldots, f_m$ and $\sum_{j=1}^m f_j$ are not lost when going from one generation to the next. We also replaced the bottom 10% of the population by random individuals. This enables the introduction of seeds to optimal solutions that may have been missing in the initial population.

3. Optimization of a solar thermal collector

We can apply now the multi-objective genetic algorithm to the optimization of a solar thermal collector. In a previous work by Gaouyat et al.,[9, 10] a flat aluminium substrate with NiCrO$_x$ and anti-reflection (AR) coatings was studied with the objective of developing high-performance solar thermal collectors. The NiCrO$_x$ ceramic-metal (cermet) composite was chosen because of its high durability and attractive absorption/emission selectivity.[3] It was shown that NiCrO$_x$ is an ideal candidate for the development of efficient solar thermal collectors.

In order to build an efficient solar thermal collector, we need to (i) maximize the solar absorptance $\alpha$ and (ii) minimize the thermal emittance $\varepsilon$.[9, 10] These quantities are defined by

$$\alpha = \int_0^\infty [1 - R(\lambda)] B_S(\lambda) d\lambda / \int_0^\infty B_S(\lambda) d\lambda \quad \text{and} \quad \varepsilon = \int_0^\infty [1 - R(\lambda)] B_S(\lambda) d\lambda / \int_0^\infty B(\lambda) d\lambda,$$

where $B_S(\lambda)$ is the solar irradiance spectrum (Air Mass 1.5), $B_S(\lambda)$ is the black-body spectrum of the absorber at 373 K and $R(\lambda)$ is the reflectance of the system for a radiation of wavelength $\lambda$ at normal incidence. $\alpha$ represents the fraction of the solar irradiance spectrum ($B_S$) that is effectively absorbed by the system. $\varepsilon$ represents the fraction of the absorber black-body spectrum ($B_\lambda$) that will escape the system (equivalent of thermal losses).

Values of $\alpha = 91.2\%$ and $\varepsilon = 1.5\%$ were achieved in a previous work by considering a bi-layer stack of NiCrO$_x$/AR deposited on a flat Al substrate.[10] We seek at improving this result by considering a waffle-shaped structuration of the substrate (see Fig. 1). We take SnO$_2$ as material for the anti-reflection coating. The geometrical parameters that characterize the Al substrate are the period $P$, the height $H$ of the holes, the ratio $f$ between the width $L$ of the holes...
on the upper side and the period \((f = L/P)\), and finally the ratio \(r\) between the width \(l\) of the holes on the bottom side and the width \(L\) of the holes on the upper side \((r = l/L)\). Conformal coatings of NiCrO\(_x\) (thickness \(t_1\)) and SnO\(_2\) (thickness \(t_2\)) are then added to this structure.

The optical properties of this waffle-shaped Al/NiCrO\(_x\)/SnO\(_2\) system were simulated by the Rigorous Coupled-Waves Analysis method for the calculation of \(R(\lambda)\).[21, 22] The optical properties of the different materials were taken from the literature and UV-visible and IR ellipsometric measurements.[8, 9, 23] We then used the multi-objective genetic algorithm to determine optimal geometrical parameters. The objective function had two components: \(f_1 = \alpha\) and \(f_2 = 1 - \varepsilon\) (\(\alpha\) must be maximized; \(\varepsilon\) must be minimized). There were six parameters to determine: \(P\), \(H\), \(f\), \(r\), \(t_1\) and \(t_2\). We considered \(P\) values between 500 and 1500 nm (step of 5 nm) and \(H\) values between 500 and 2500 nm (step of 5 nm). These boundaries left \(P\) and \(H\) in the same range as the incident wavelengths. We took \(f\) between 0.5 and 0.99 (step of 0.01) and \(r\) between 0 and 0.99 (step of 0.01) in order to explore the full range of inverted pyramidal shapes. We took finally \(t_1\) and \(t_2\) between 50 nm and 100 nm (step of 5 nm) in order to be representative of layer thicknesses obtained by physical vapor deposition (PVD). These parameter specifications left us with 48,763,605,000 possibilities to explore. Only 2377 evaluations of the fitness were however required by the GA.

Fig. 2 shows that the genetic algorithm progressively established a whole set of Pareto-optimal solutions. The number of these solutions increases indeed progressively to 70 on average after 30 generations. These solutions all provide \((f_1, f_2)\) values with a distinct advantage compared to the rest of the population. No individual in the whole population provides indeed better values for both \(f_1\) and \(f_2\). Amongst this set of Pareto-optimal solutions, individuals that are better for \(f_1\) are necessarily weaker for \(f_2\). This is illustrated in Table 1, where a selection of Pareto-optimal solutions is provided. Table 1 also provides the solution that maximizes \(f_1 + f_2\).

These results compare very well with the values of \(\alpha=91.2\%\) and \(\varepsilon=1.5\%\) achieved in previous work with a flat Al/NiCrO\(_x\)/AR configuration[10] and with the record values of \(\alpha=97\%\) and \(\varepsilon=5\%\) obtained on a 3-layers stack.[8] The calculation accounts not only for the enhancement of \(\alpha\), but also for the combined optimization of both \(\alpha\) and \(\varepsilon\). The higher values achieved for the absorptance \(\alpha\) are coupled with an increase of the emittance \(\varepsilon\). The optimization process deals indeed with the cut-off wavelength \(\lambda_c\) at which the reflectance goes essentially from zero to one. A shift of \(\lambda_c\) to higher wavelengths leads to an increase of both \(\alpha\) and \(\varepsilon\) (see the defi-
Fig. 2. Left: number of Pareto-optimal solutions when searching for \( P, H, f, r, t_1 \) and \( t_2 \) with the objective of optimizing the parameters \( \alpha \) and \( \varepsilon \) of a solar thermal collector; Right: reflectance spectrum of the waffle-shaped Al/NiCrO\(_x\)/SnO\(_2\) structure that provides \( \alpha = 97.8\% \) and \( \varepsilon = 4.8\% \) (solid), a flat Al/NiCrO\(_x\)/SnO\(_2\) structure with \( t_1 = t_2 = 50 \) nm (dashed) and a flat uncoated Al (dot-dashed). The figure includes the normalized solar irradiance spectrum \( B_S(\lambda) \) and the normalized black-body spectrum \( B_a(\lambda) \) of the absorber at 373 K.

\[
\begin{array}{cccccccc}
P (\text{nm}) & H (\text{nm}) & f & r & t_1 (\text{nm}) & t_2 (\text{nm}) & \alpha & \varepsilon \\
1345 & 1960 & 0.96 & 0.45 & 50 & 50 & 97.8\% & 4.8\% \\
1435 & 1975 & 0.99 & 0.31 & 55 & 50 & 98.4\% & 5.8\% \\
795 & 1590 & 0.90 & 0.28 & 50 & 50 & 96.1\% & 4.1\% \\
560 & 545 & 0.95 & 0.28 & 50 & 50 & 95.2\% & 3.7\% \\
\end{array}
\]

Table 1. Parameters relevant to the optimization of \( \alpha \) and \( \varepsilon \) of a solar thermal collector. The first line corresponds to the solution that maximizes \( f_1 + f_2 \). The next three lines correspond to selected Pareto-optimal solutions.

Definitions of \( \alpha \) and \( \varepsilon \) and the representations of \( B_S(\lambda) \) and \( B_a(\lambda) \) in Fig. 2. This increase of the emittance \( \varepsilon \) to values that stay below 5.8% for the solutions presented in Table 1 is however low enough to maintain strong performances.

The solution that provides the maximal value for \( f_1 + f_2 \) gives absorptance and emittance values of \( \alpha = 97.8\% \) and \( \varepsilon = 4.8\% \). The reflectance \( R(\lambda) \) associated with this solution is shown in Fig. 2. The figure includes for comparison the reflectance spectrum of a flat uncoated Al as well as the reflectance spectrum of a flat Al/NiCrO\(_x\)/SnO\(_2\) stack with \( t_1 = t_2 = 50 \) nm. These results confirm that the cermet and anti-reflection coatings play their role in reducing significantly the reflectance \( R(\lambda) \) in the main part of the solar spectrum \( B_S(\lambda) \). This explains the high values of \( \alpha, R(\lambda) \) then increases rapidly to values that are close to 1 for the main part of the absorber black-body spectrum \( B_a(\lambda) \). This explains the small values of \( \varepsilon \).

As the solar and black-body spectra only slightly overlap, a conjoint optimization of both the solar absorptance \( \alpha \) and the thermal emittance \( \varepsilon \) was indeed possible. The transition in the reflectance must however be sharp and located at a wisely chosen cut-off wavelength \( (\lambda_c) \). This cut-off wavelength depends on the black-body temperature because of optimization considerations.[2] The ideal reflectance curve of a solar absorber is represented in Fig. 4 of Ref. [2]. It indicates a cut-off wavelength \( \lambda_c \) at around 2.5 \( \mu \text{m} \), for a 373 K black-body temperature. With the addition of the underlying structure, the cut-off wavelength observed in Fig. 2 with our Al/NiCrO\(_x\)/SnO\(_2\) configuration has shifted from 1.5 \( \mu \text{m} \) to 2.5 \( \mu \text{m} \) indeed. The shift of \( \lambda_c \) to longer wavelengths leads to a strong increase of the solar absorptance \( \alpha \). It also leads to a slight increase of the thermal emittance \( \varepsilon \). Emittance values of the order of 5% are however
tolerable as they do not spoil performances.

The comparison between the flat and waffle-shaped Al/NiCrO$_x$/SnO$_2$ configurations proves that the patterning of the Al substrate has a significant impact on the reflectance spectrum and therefore on the absorptance $\alpha$ and the emittance $\varepsilon$. Values of $\alpha = 84.9\%$ and $\varepsilon = 1.7\%$ are indeed obtained with the flat Al/NiCrO$_x$/SnO$_2$ configuration (taking $t_1=t_2=50$ nm), while values of $\alpha = 97.8\%$ and $\varepsilon = 4.8\%$ are obtained with the waffle-shaped configuration. The solutions listed in Table 1 represent different alternatives for the realization of a high-performance solar thermal collector. The optimization significantly enhanced the solar absorptance $\alpha$ with a reasonably moderate increase of the thermal emittance $\varepsilon$, hence reaching the expected record performances. Making a choice between these different solutions will depend on the trade-off we want to have between $\alpha$ and $\varepsilon$ and on other practical issues.

4. Conclusion

We applied a multi-objective genetic algorithm to the optimization of a solar thermal collector that consists of a waffle-shaped Al substrate with NiCrO$_x$ and SnO$_2$ conformal coatings. This problem involved the determination of optimal geometrical parameters in order to (i) maximize the solar absorptance $\alpha$ and (ii) minimize the thermal emittance $\varepsilon$. By using a multi-objective genetic algorithm, we actually obtained a whole set of Pareto-optimal solutions. These solutions represent different alternatives for the realization of a collector, the choice of a particular solution depending on a trade-off between $\alpha$ and $\varepsilon$. The values of $\alpha = 97.8\%$ and $\varepsilon = 4.8\%$ achieved in this work turn out to be competitive with record values found in the literature. Approaching this problem by a systematic scan on parameters would have been untractable considering the huge number of possibilities (48,763,605,000) and the time required for each evaluation of the fitness (up to 30 hours on a supercalculator). The genetic algorithm could however address this problem by evaluating in parallel only a reduced number of possibilities. This proves the interest of multi-objective genetic algorithms for addressing complex optimization problems in physics.

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Appendix: Effective fitness based on a Pareto-classification of the population

We define in this Appendix the effective fitness $f_{\text{eff}}$ that was used with the multi-objective genetic algorithm.[20] We refer as previously by $n_{\text{pop}}$ to the size of the population, by $n$ to the number of parameters $x_i$ and by $m$ to the number of components $f_j$ of the objective function. Pareto-optimal solutions were defined as solutions that are not dominated. They receive a rank of 1. Solutions that are only dominated by solutions of rank 1 receive a rank of 2. Solutions of rank 3 are only dominated by solutions of rank 1 and 2. We can proceed in this way and attribute a rank to the whole population. The effective fitness $f_{\text{eff}}$ must be higher for individuals
of lower rank if we want the GA to search for Pareto-optimal solutions.

We proceed therefore in the following way to define the effective fitness: all individuals of rank 1 receive an effective fitness of \( n_{\text{pop}} \). We then define a sharing function in order to reduce, amongst individuals of the same rank, the effective fitness of individuals that are too close from each other. This will indeed avoid early convergence of the GA to a given individual. For individuals of the same rank, we define a distance matrix whose components are defined by

\[
d_{k,l} = \sqrt{\sum_{i=1}^{n} (x_i[k] - x_i[l])^2 / (x_i^{\text{max}} - x_i^{\text{min}})^2},
\]

where \( x_i[k] \) refers to the parameter \( x_i \) of an individual \( k \), \( x_i^{\text{max}} = \max_{k \in [1,n_{\text{pop}}]} x_i[k] \) and \( x_i^{\text{min}} = \min_{k \in [1,n_{\text{pop}}]} x_i[k] \). The sharing function between two individuals is then defined by

\[
S_{k,l} = 1 - \left( \frac{d_{k,l}}{\sigma_{\text{share}}} \right)^2 \text{ if } d_{k,l} \leq \sigma_{\text{share}} \text{ and } 0 \text{ otherwise.}
\]

Following Refs [19, 20], we take \( \sigma_{\text{share}} = 0.5 \sqrt{\frac{1}{10}} \). We then define the niche count of a given individual by

\[
m_k = \sum_l S_{k,l},
\]

where the sum is restricted to individuals of the same rank. The effective fitness of each individual is finally divided by its niche count. The effective fitness of all individuals of rank 2 is then initialized with a value of \( 0.99 \times f_{\text{eff},\text{min}} [\text{rank 1}] \), where \( f_{\text{eff},\text{min}} [\text{rank 1}] \) refers to the minimal value of the effective fitness for the individuals of rank 1. We proceed by computing the distance matrix \( d_{k,l} \), the sharing function \( S_{k,l} \) and the niche count \( m_k \) for all individuals of rank 2. Their effective fitness is then divided by their niche count. We continue in this way until the whole population has been attributed an effective fitness.