

RESEARCH OUTPUTS / RÉSULTATS DE RECHERCHE

Multi-objective genetic algorithm for the optimization of a flat-plate solar thermal collector

Mayer, Alexandre; Gaouyat, Lucie; Nicolay, Delphine; Carletti, Timoteo; Deparis, Olivier

Published in:
Optics Express

DOI:
[10.1364/OE.22.0A1641](https://doi.org/10.1364/OE.22.0A1641)

Publication date:
2014

Document Version
Early version, also known as pre-print

[Link to publication](#)

Citation for published version (HARVARD):
Mayer, A, Gaouyat, L, Nicolay, D, Carletti, T & Deparis, O 2014, 'Multi-objective genetic algorithm for the optimization of a flat-plate solar thermal collector', *Optics Express*, vol. 22, no. 21, pp. A1641-A1649.
<https://doi.org/10.1364/OE.22.0A1641>

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal ?

Take down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

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

Alexandre Mayer^{1,*}, Lucie Gaouyat¹, Delphine Nicolay², Timoteo Carletti² and Olivier Deparis¹

¹Laboratoire de Physique du Solide, University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium

² Department of Mathematics, University of Namur, Rempart de la Vierge 8, 5000 Namur, Belgium

*alexandre.mayer@unamur.be

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 SnO₂ anti-reflection conformal coatings. Optimal geometrical parameters are determined in order to (i) maximize the solar absorptance α and (ii) minimize the thermal emittance ε . The multi-objective genetic algorithm eventually provides a whole set of Pareto-optimal solutions for the optimization of α and ε , 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.

© 2014 Optical Society of America

OCIS codes: (350.6050) Solar energy; (310.6845) Thin film devices and applications; (350.4600) Optical engineering; (000.3860) Mathematical methods in physics.

References and links

1. X.-F. Li, Y.-R. Chen, J. Miao, P. Zhou, Y.-X. Zheng, L.-Y. Chen, and Y.-P. Lee, "High solar absorption of a multilayered thin film structure," *Opt. Express* **15**(4), 1907–1912 (2007).
2. F. Cao, K. McEnaney, G. Chen, and Z. Ren, "A review of cermet-based spectrally selective solar absorbers," *Energy Environ. Sci.* **7**, 1615–1627 (2014).
3. C.E. Kennedy, "Review of Mid- to High-Temperature Solar Selective Absorber Materials," NREL/TP-520-31267, National Renewable Energy Laboratory, Colorado, July 2002.
4. R.A. Buhrman, "Physics of solar selective surfaces," in *Physics of solar selective surfaces*, K.W. Böer, ed. (Springer, 1986), vol. 3, chap. 4.
5. T. Boström, E. Wäckelgård, and G. Westin, "Solution chemical route to nickel-alumina coatings for thermal solar absorbers," *Sol. Energy* **74**, 497–503 (2003).
6. V. Teixeira, E. Sousa, M.F. Costa, C. Nunes, L. Rosa, and M.J. Carvalho, "Spectrally selective composite coatings of Cr-Cr₂O₃ and Mo-Al₂O₃ for solar energy applications," *Thin Solid Films* **392**, 320–326 (2001).
7. S. Zhao and E. Wäckelgård, "The optical properties of sputtered composite of Al-AlN," *Sol. Energ. Mat. Sol. C.* **90** (13), 1861–1874 (2006).
8. S. Zhao and E. Wäckelgård, "Optimization of solar absorbing three-layer coatings," *Sol. Energ. Mat. Sol. C.* **90**(3), 243–261 (2006).
9. L. Gaouyat, F. Mirabella, and O. Deparis, "Critical tuning of magnetron sputtering process parameters for optimized solar selective absorption of NiCrOx cermet coatings on aluminium substrate," *Appl. Surf. Sci.* **271**, 113–117 (2013).
10. L. Gaouyat, Z. He, J.-F. Colomer, Ph. Lambin, F. Mirabella, D. Schryvers, and O. Deparis, "Revealing the innermost nanostructure of sputtered NiCrOx solar absorber cermets," *Sol. Energ. Mat. Sol. C.* **122**, 303–308 (2014).
11. D. Chester, P. Bermel, J.D. Joannopoulos, M. Soljacic, I. Celanovic, "Design and global optimization of high-efficiency solar thermal systems with tungsten cermets," *Opt. Express* **19** (53), A245–A257 (2011).

12. A. Lasagni, M. Nejati, R. Clasen, and F. Mücklich, "Periodic surface structuring of metals by laser interference metallurgy as a new fabrication method of textured solar selective absorbers," *Adv. Eng. Mater.* **8** (6), 580–584 (2006).
 13. M. Shimizu, K. Takeuchi, H. Sai, F. Iguchi, N. Sata, and H. Yugami, "High-temperature solar selective absorber material using surface microcavity structures," *Proc. ASME* **5**, 783–787 (2011).
 14. J.H. Holland, *Adaptation in Natural and Artificial Systems* (University of Michigan Press, 1975).
 15. K.A. De Jong, *An analysis of the behaviors of genetic adaptive systems*, PhD thesis (University of Michigan, 1975).
 16. D.E. Goldberg, *Genetic Algorithms in Search, Optimization and Machine Learning* (Addison-Wesley, 1989).
 17. R. Judson, "Genetic Algorithms and their use in Chemistry," in *Reviews in Computational Chemistry*, K.B. Lipkowitz and D.B. Boyd, ed. (VCH Publishers, 1997), vol. 10, chap. 1.
 18. R.L. Haupt and D.H. Werner, *Genetic Algorithms in Electromagnetics* (Wiley&Sons, 2007).
 19. K. Deb, "Multi-objective evolutionary algorithms: Introducing bias among Pareto-optimal solutions," in *Advances in Evolutionary Computing* (Springer-Verlag, 2003), pp. 263–292.
 20. D. Nicolay, *Modélisation et apprentissage des réseaux de neurones artificiels*, Master thesis (University of Namur, 2012).
 21. J.-P. Vigneron, F. Forati, D. André, A. Castiaux, I. Derycke, and A. Dereux, "Theory of electromagnetic energy transfer in three-dimensional structures," *Ultramicroscopy* **61**, 21–27 (1995).
 22. J.-P. Vigneron and V. Lousse, "Variation of a photonic crystal color with the miller indices of the exposed surface," *Proc. SPIE* 6128, 61281G (2006).
 23. O. Stenzel, *The Physics of Thin Film Optical Spectra: An Introduction* (Springer, 2005).
-

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] cermet, in the form of thin films, are today the only industrial alternative. Cermet is 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-Al₂O₃, Cr-Cr₂O₃, 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, cermet is 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 α and the thermal emittance ε . 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 α should be maximized and the thermal emittance ε should be minimized. We hence need to conjointly optimize α and ε 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 SnO₂), but also the geometrical parameters

of the waffle-like structure.

Nature has developed its own algorithms for determining optimal solutions. With genetic algorithms (GA), we actually mimic natural selection in order to determine the optimal parameters of complex problems in physics.[14, 15, 16] The idea consists in working with a population of individuals, each of them representing a given set of physical parameters. The initial population usually consists of random individuals. The best individuals are then selected. They generate new individuals for the next generation. Random mutations in the coding of parameters are finally introduced. When applied from generation to generation, this evolutionary strategy makes it possible to determine the global optimum of a problem. These general principles actually leave room for a variety of interpretations regarding the way a genetic algorithm should be implemented.[17, 18] There are indeed different ways to assign a fitness to each individual, different strategies for the selection, different methods for the crossing and mutation 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_x and SnO₂ conformal coatings. The geometrical parameters of this system must be adjusted in order to achieve two objectives: (i) to maximize the absorptance α and (ii) to minimize the emittance ε . 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 $\vec{f} = \vec{f}(\vec{x})$ be an objective function of m components $f_1(\vec{x}), \dots, f_m(\vec{x})$. Each component $f_j(\vec{x})$ depends on n physical parameters x_i , where $x_i \in [x_i^{\min}, x_i^{\max}]$ with a specified granularity of Δx_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 $(x_i^{\max} - x_i^{\min}) / (2^{n_i} - 1) \leq \Delta x_i$. The value of the physical parameter x_i is then given by $x_i = x_i^{\min} + \langle \text{gene } i \rangle \times \Delta x_i$, where $\langle \text{gene } i \rangle \in [0, 2^{n_i} - 1]$ stands for the value coded by the gene i in Gray binary coding.[17] The genetic algorithm must reject gene values that lead to $x_i > x_i^{\max}$ in order to achieve a strict enforcement of our parameter specifications. A given set of parameters $\{x_i\}_{i=1}^n$ 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 $\{x_i\}_{i=1}^n$. The initial population usually consists of random individuals. These individuals must be evaluated in order to determine the corresponding values of the objective function \vec{f} . We must also define an effective fitness f_{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 f_{eff} that depends on the *Pareto-classification* of these individuals.[18, 19, 20] 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_{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_{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, \dots, 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 α and (ii) minimize the thermal emittance ε . [9, 10] These quantities are defined by $\alpha = \int_0^\infty [1 - R(\lambda)] B_S(\lambda) d\lambda / \int_0^\infty B_S(\lambda) d\lambda$ and $\varepsilon = \int_0^\infty [1 - R(\lambda)] B_a(\lambda) d\lambda / \int_0^\infty B_a(\lambda) d\lambda$, where $B_S(\lambda)$ is the solar irradiance spectrum (Air Mass 1.5), $B_a(\lambda)$ 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 λ at normal incidence. α represents the fraction of the solar irradiance spectrum (B_S) that is effectively absorbed by the system. ε represents the fraction of the absorber black-body spectrum (B_a) 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 SnO₂ 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.

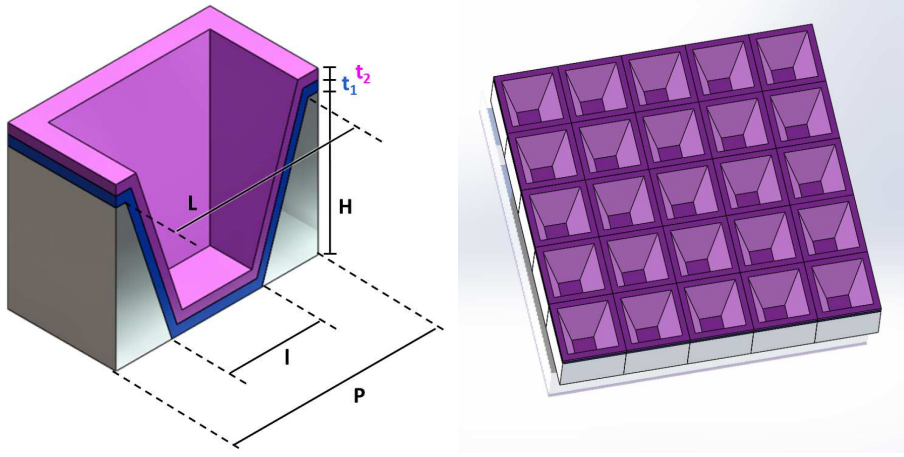


Fig. 1. Waffle-shaped Al substrate with NiCrO_x and SnO_2 conformal coatings. This structure is considered for the development of high-performance solar thermal collectors.

The optical properties of this waffle-shaped $\text{Al}/\text{NiCrO}_x/\text{SnO}_2$ 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 $f_2 = 1 - \varepsilon$ (α must be maximized; ε 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 $\text{Al}/\text{NiCrO}_x/\text{AR}$ 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 α , but also for the combined optimization of both α and ε . The higher values achieved for the absorptance α are coupled with an increase of the emittance ε . The optimization process deals indeed with the cut-off wavelength λ_c at which the reflectance goes essentially from zero to one. A shift of λ_c to higher wavelengths leads to an increase of both α and ε (see the defi-

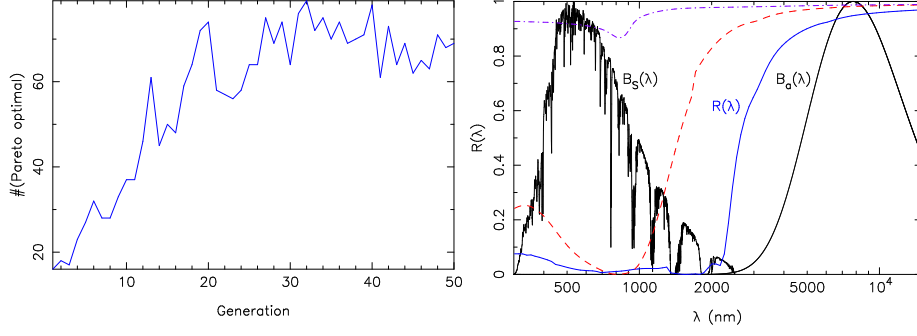


Fig. 2. Left: number of Pareto-optimal solutions when searching for P , H , f , r , t_1 and t_2 with the objective of optimizing the parameters α and ε of a solar thermal collector; Right: reflectance spectrum of the waffle-shaped Al/NiCrO_x/SnO₂ structure that provides $\alpha = 97.8\%$ and $\varepsilon = 4.8\%$ (solid), a flat Al/NiCrO_x/SnO₂ 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.

P (nm)	H (nm)	f	r	t_1 (nm)	t_2 (nm)	α	ε	
1345	1960	0.96	0.45	50	50	97.8%	4.8%	$f_1 + f_2$ max
1435	1975	0.99	0.31	55	50	98.4%	5.8%	P-optimal
795	1590	0.90	0.28	50	50	96.1%	4.1%	P-optimal
560	545	0.95	0.28	50	50	95.2%	3.7%	P-optimal

Table 1. Parameters relevant to the optimization of α and ε 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.

nitions of α and ε and the representations of $B_S(\lambda)$ and $B_a(\lambda)$ in Fig. 2). This increase of the emittance ε 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/SnO₂ 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 α . $R(\lambda)$ 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 ε .

As the solar and black-body spectra only slightly overlap, a conjoint optimization of both the solar absorptance α and the thermal emittance ε was indeed possible. The transition in the reflectance must however be sharp and located at a wisely chosen cut-off wavelength (λ_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 λ_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/SnO₂ configuration has shifted from $1.5 \mu\text{m}$ to $2.5 \mu\text{m}$ indeed. The shift of λ_c to longer wavelengths leads to a strong increase of the solar absorptance α . It also leads to a slight increase of the thermal emittance ε . 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/SnO₂ configurations proves that the patterning of the Al substrate has a significant impact on the reflectance spectrum and therefore on the absorptance α and the emittance ε . Values of $\alpha = 84.9\%$ and $\varepsilon = 1.7\%$ are indeed obtained with the flat Al/NiCrO_x/SnO₂ 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 α with a reasonably moderate increase of the thermal emittance ε , hence reaching the expected record performances. Making a choice between these different solutions will depend on the trade-off we want to have between α and ε 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 SnO₂ conformal coatings. This problem involved the determination of optimal geometrical parameters in order to (i) maximize the solar absorptance α and (ii) minimize the thermal emittance ε . 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 α and ε . 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.

Acknowledgements

A.M. is funded by the Fund for Scientific Research (F.R.S.-FNRS) of Belgium. L.G. is supported by FNRS-FRIA. D.N. and T.C. acknowledge the Belgian Network DYSCO (Dynamical Systems, Control, and Optimization), funded by the Interuniversity Attraction Poles Programme and initiated by the Belgian Science Policy Office. A.M, D.N. and T.C. are members of naXys, Namur Center for Complex Systems. This research used resources of the "Plateforme Technologique de Calcul Intensif (PTCI)" (<http://www.ptci.unamur.be>) located at the University of Namur, Belgium, which is supported by the F.R.S.-FNRS under the convention No. 2.4520.11. The PTCI is member of the "Consortium des Equipements de Calcul Intensif (CECI)" (<http://www.ceci-hpc.be>). Erwin Volon is acknowledged for his Solid Works representations of the Al/NiCrO_x/SnO₂ structure.

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

We define in this Appendix the effective fitness f_{eff} that was used with the multi-objective genetic algorithm.[20] We refer as previously by n_{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_{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_{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 $d_{k,l} = \sqrt{\sum_{i=1}^n (x_i[k] - x_i[l])^2 / (x_i^{\max} - x_i^{\min})^2}$, where $x_i[k]$ refers to the parameter x_i of an individual k , $x_i^{\max} = \max_{k \in [1, n_{\text{pop}}]} x_i[k]$ and $x_i^{\min} = \min_{k \in [1, n_{\text{pop}}]} x_i[k]$. The sharing function between two individuals is then defined by $S_{k,l} = 1 - (d_{k,l} / \sigma_{\text{share}})^2$ if $d_{k,l} \leq \sigma_{\text{share}}$ and 0 otherwise. Following Refs [19, 20], we take $\sigma_{\text{share}} = 0.5 / \sqrt[10]{n}$. 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 $0.99 \times f_{\text{eff},\min}[\text{rank } 1]$, where $f_{\text{eff},\min}[\text{rank } 1]$ 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.