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# Optimization of a perfect absorber multilayer structure by genetic algorithms

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## Abstract

**Background:** An increasing interest has been recently grown in the development of nearly perfect absorber materials for solar energy collectors and more in general for all the thermophotovoltaic applications.

**Methods:** Wide angle and broadband perfect absorbers with compact multilayer structures made of a sequence of ITO and TiN layers are here studied to develop new devices for solar thermal energy harvesting. Genetic Algorithms are introduced for searching the optimal thicknesses of the layers so to design a perfect broadband absorber in the visible range, for a wide range of angles of incidence from 0° to 50°, and for both polarizations.

**Results:** Genetic Algorithms allow to design several optimized structures with 6, 8, and 10 layers reaching a very high average absorbance of 97%, 99% and 99.5% respectively together with a low hemispherical total emissivity (<20%) from 200 °C till 400 °C.

**Conclusions:** The proposed multilayer structures use materials with high thermal stability, and high melting temperature, can be fabricated with simple thin film deposition techniques, appearing to have very promising applications in solar thermal energy harvesting.

**Keywords:** Optical materials and properties, Perfect absorber, Multilayer structure, Thermophotovoltaic, Solar energy collectors

## Background

During last decade a huge interest has been grown in the development of nearly perfect absorber materials for applications as solar energy collectors, and, more in general, for all the thermophotovoltaic applications (TPV), so to increase the absorbed power for energy harvesting, storage and conversion as well as for the reprocessing of wasted heat in industrial processes [1, 2].

The use of carbon nanotube technology improved a lot the performance of the absorbing materials. In 2009 nanomaterials based on vertically aligned single-walled carbon nanotubes shown an absorbance of about 98% of the incoming light in a wide spectral range UV-VIS-NIR [3]. But despite recent advances in the development of carbon nanotubes (CNT) purity assessment tools, the macroscale assessment of the overall surface qualities of commercial CNT materials remains a great challenge,

bringing negative impacts on the reliable and consistent nano-manufacturing of CNT products [4, 5].

A new concept of perfect absorber is now based on metamaterials where the enhancement of the absorption can be obtained thanks to the excitation of the surface plasmon resonance for example in gold and silver [6–13]. This can be achieved with structured metallic surfaces [14], microcavities [15], subwavelength hole arrays and opals [16, 17]. Alternatively structured phase change materials [18–23] and chiral metamaterials [24–27] have been recently used so to obtain an active switching of the absorption properties thanks to the metal-insulator transition in one case, or to intrinsic/extrinsic dichroism in the other case. However, the realisation of broadband absorber metamaterials requires long and expensive procedures with multiple steps of film deposition, photoresist coating, etching and photoresist removing [28].

It should be underlined that the design and realisation of perfect absorbers with multilayers can be more technically and economically convenient [29]. The multilayer structure can be easily theoretically tested by numerical

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simulations, and optimized so to obtain broadband absorbers for a wide range of angles of incidence by using several standard search methods (Genetic Algorithms [30], Neural Network [31–33], Singular Value Decomposition [34–36], Steepest Descent Methods [37, 38], etc...). In addition the multilayered opaque structures are also easy to be characterized by using many different diagnostic techniques: photothermal, photoacoustic, photopyroelectric, and thermographic techniques [39–45].

Concerning the materials, an increasing interest is for the inorganic ceramic materials such as semiconductor-based oxides and transition-metal nitrides (TiN) which represent the alternative plasmonic materials in the visible frequencies [46–50], with a good thermal stability [51, 52].

Other common materials for optical electronic device applications and solar cells are the transparent conducting oxides (i.e. ITO) which can support surface plasmon polariton excitations [53, 54].

In this paper we study and optimize a multilayer structure based on a stack of ITO/TiN layers deposited onto a silver thick layer so to design the coating of a solar thermal collector. The idea of such a structure has been recently proposed in Ref. [49]. The authors designed an ITO/TiN multilayer finding an average absorbance of 90% in the visible for a wide range of incidence angle with 7 layers but without studying the infrared emissivity. Our purpose is to optimize this configuration by introducing a silica top layer in order to reach a higher average absorbance and by analysing the low thermal emissivity properties of the structure at different temperatures. We performed numerical simulations by changing the number of layers, and the layer thicknesses, and we applied the Genetic Algorithms to find the optimal thicknesses of the multilayer structure.

## Methods

In this section we discuss the approach to design a ITO/TiN multilayered structure to be an efficient coating for solar thermal collectors. The structure will be designed so to exhibit the highest average absorbance in the

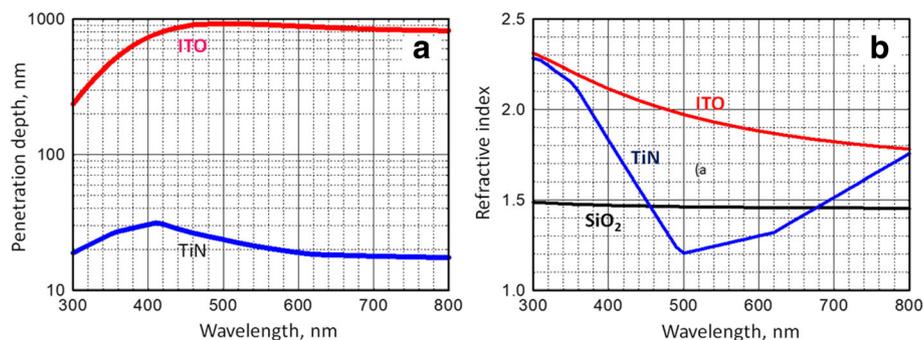
spectral range from 400 nm to 750 nm (visible window) for a wide range of incidence angles from  $0^\circ$  to  $50^\circ$ , but also satisfying the requirement on a low thermal emissivity ( $< 20\%$ ) in the infrared, so to minimize the radiative losses of the solar collector.

The concept of multiband perfect absorbers by using metallo/dielectric multilayers has been recently introduced [55, 56]. It is known that 1D Photonic Band Gap structures can be tailored for specific photonic devices to exhibit exceptional properties, for example to obtain the transparency in metals [57–60], as well as to achieve the total absorbance [55] in a wide range of wavelengths. Regarding the perfect absorbance, metallo/dielectric structures can fulfill three important requirements at the same time, when a large number of layers is applied:

- to act as antireflection coating so to minimize the sample reflectance in the visible [56–59];
- to maximize the absorbance in the metallic layers;
- to guarantee a low thermal emissivity in the infrared thanks to the metal layers.

Starting from this state of the art, we want to show that it is possible to achieve better results by replacing the metal layers with Titanium Nitride layers (TiN) [50].

In fact TiN is an inexpensive metal alloy with smaller free carrier concentrations than noble metals. It behaves as a diluted metal but with material losses comparable to that of gold, showing an optical penetration depth of about 20–30 nm, in the visible range (see Fig. 1a obtained from the data in ref. [61]). In addition TiN has also good mechanical hardness, high corrosion resistance, low frictional constant, thermodynamic stability, relatively good thermal conductivity ( $\approx 20$  W/m K), low thermal emissivity ( $< 0.2$ ), very high melting temperature of  $2930^\circ\text{C}$ , and a thermal expansion of  $9.3 \times 10^{-6} \text{ K}^{-1}$  that is lower than for gold ( $14 \times 10^{-6} \text{ K}^{-1}$ ) and silver ( $18 \times 10^{-6} \text{ K}^{-1}$ ). These properties makes it suitable for applications such as thermal radiation engineering and thermophotovoltaics [62, 63].

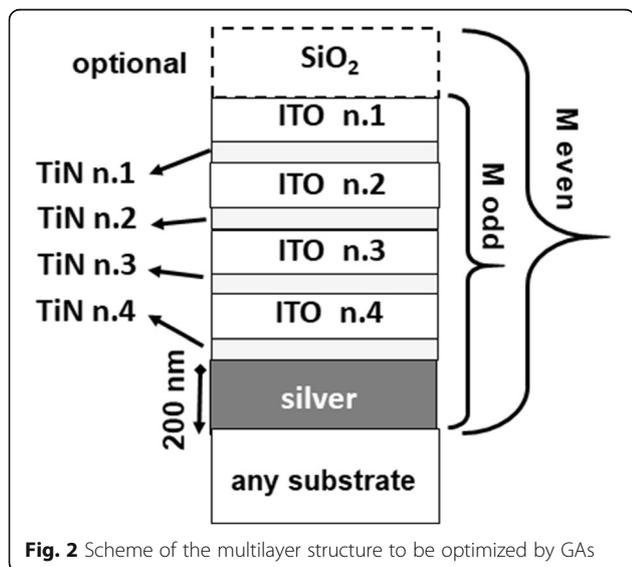


**Fig. 1** Penetration depth (a) and refractive index (b) as a function of wavelength in the visible range for ITO, TiN, and  $\text{SiO}_2$ . Penetration depth for silica is not shown because is highly transparent

In our case the TiN layers are alternated with transparent Indium tin oxide layers (ITO) so to design the ITO/TiN multilayer structure made of  $M$  layers as shown in Fig. 2. ITO is a transparent conductive oxide, widely used in electronic and optical devices, and compatible with TiN during the deposition process. ITO shows a sufficiently large optical penetration depth of about 700–1000 nm in the visible (see Fig. 1a [64]), with a high refractive index (see Fig. 1b) in the visible, high melting point ( $> 1500$  °C), and relatively low thermal emissivity.

An earlier study concerning the combination of these two materials has already shown how the average absorbance can reach 90% in the visible and for a wide range of incidence angles by using only 7 layers [49]. However we show here that this scheme can be further improved by introducing a silica top layer which acts as an additional antireflection coating (being  $n_{SiO_2} \cong \sqrt{n_{ITO} \cdot n_{air}}$ ), without any relevant increase of the thermal emissivity, (see Fig. 1b), and by searching the optimal thicknesses of the whole structure with Genetic Algorithms (GAs).

GAs have been introduced in the 60s by John Holland for two purposes [65]: to explain the adaptive processes of natural systems, and to design artificial systems software capable to emulate the mechanisms of natural systems. For many years GAs have been applied to solve both optimization and inverse problems in many different scientific fields: in biology [66, 67] in computer science [68, 69], in engineering and physics for adaptive filter design [70], in the synthesis of fiber gratings, in thin film metrology [71], in image processing [72], and in metallurgy for the nondestructive testing (NDT) of materials [73–75].



Adopting the terminology of the biological sciences, GAs evaluate, process and manipulate a population of *chromosomes* that represent possible solutions in the research space. In our case the chromosome is a string containing the values of the layer thicknesses of the ITO/TiN structure: for example for  $M$  layers, the chromosome is a string containing  $M$  genes  $\{d_1, d_2, d_3, d_4, \dots, d_M\}$  where  $d_i$  is the thickness of the generic  $i$ -th layer (from top to bottom) (see Fig. 2). For each chromosome, a numerical simulation should be performed to calculate the absorbance of the multilayer by using the transfer-matrix method [76], and to quantify how much the absorbance is close to the ideal case of 100% through the *fitness* of the chromosome. Each chromosome belongs to the population of  $N_{pop}$  individuals. Thanks to the mutual interactions among individuals and to the natural selection mechanisms, the population can evolve and adapt to the environment (research domain), increasing the fitness of all individuals, and eventually finding the best chromosome representing the optimal ITO/TiN multilayer structure.

Once the approach and the methods to optimize the ITO/TiN multilayer structure have been chosen, all the constraints, the requirements and the technical details on the optimization procedure, applied to the design of a heat solar collector, should be also introduced according to the following guidelines:

- a) The structure is made of a sequence of ITO and TiN layers. The thickness for each ITO layer should be searched by GAs in the range [5 nm – 100 nm], thinner than  $\lambda/2$  so to avoid internal interference effects. Each TiN layer should be searched by GAs in the interval [5 nm – 60 nm] so to play with its transparency/opaqueness.
- b) A silica top layer can be optionally inserted as additional antireflection coating. Its thickness should be searched by GAs in the range [5 nm – 150 nm], without causing a relevant change of the IR emissivity.
- c) The last 200 nm thick silver layer absorbs and stops the residual radiation. Therefore the results of the numerical simulations and optimizations are general and independent on the choice of the substrate.
- d) The total number of layers  $M$  ranges from 3 to 10. The silica top layer is inserted only when  $M$  is an even number (see Fig. 2). The optimized multilayers found by GAs for different values of  $M$ , will be discussed and compared.
- e) The objective to be maximized is the absorbance  $A_{av}$  averaged in the visible range from  $\lambda_{min} = 400$  nm to  $\lambda_{max} = 750$  nm, and averaged for a wide range of angles of incidence from  $0^\circ$  to  $\lambda_{max} = 50^\circ$ , for unpolarised light. It is calculated as follows





**Table 4** Results after the mutation procedure applied to the population in Table 3

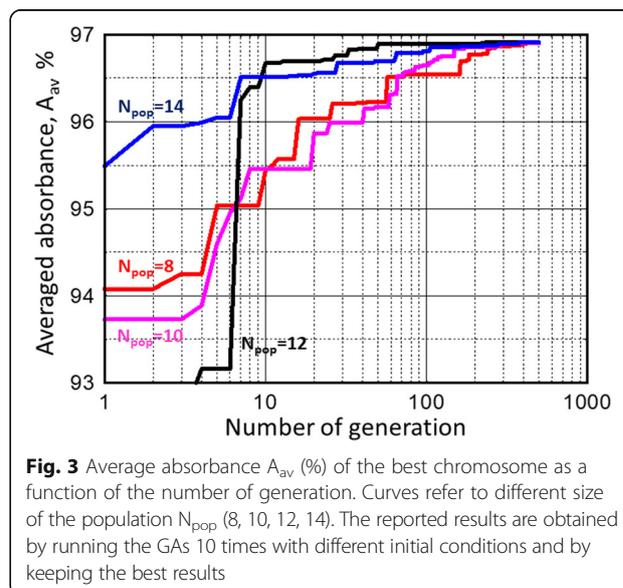
N <sub>pop</sub> Chromosomes→		1	2	3	4	5	6	7	8
A <sub>0</sub>	→	89.3	91.8	91.3	82.4	92.9	87.6	80.5	78.7
A <sub>av</sub>	→	89.2	91.6	91.9	83.1	93.0	88.4	82.0	79.6
Fitness (x 10 <sup>-6</sup> )	→	74	203	237	12	414	55	9	6
M genes	Structure	nm							
1	SiO <sub>2</sub>	49	49	85	80	65	98	85	83
2	ITO n.1	41	41	39	39	38	37	34	24
3	TiN n.1	16	16	20	38	19	24	37	34
4	ITO n.2	29	37	62	43	45	64	80	84
5	TiN n.2	58	58	48	43	53	46	38	37
6	Silver	200	200	200	200	200	200	200	200

chromosome of the population is found to be the N.6 (the column is highlighted in black in Table 1).

From Table 1 the best chromosomes are randomly selected for the reproduction with a probability proportional to the fitness value so to give more chances to the best chromosomes respect to the worst ones which risk the extinction. Table 2 shows the new population selected for the reproduction. The best chromosomes can be selected more than once so to transfer the best chromosomal strings to future generations: in fact in Table 2 there are 4 replica of the best chromosome of Table 1.

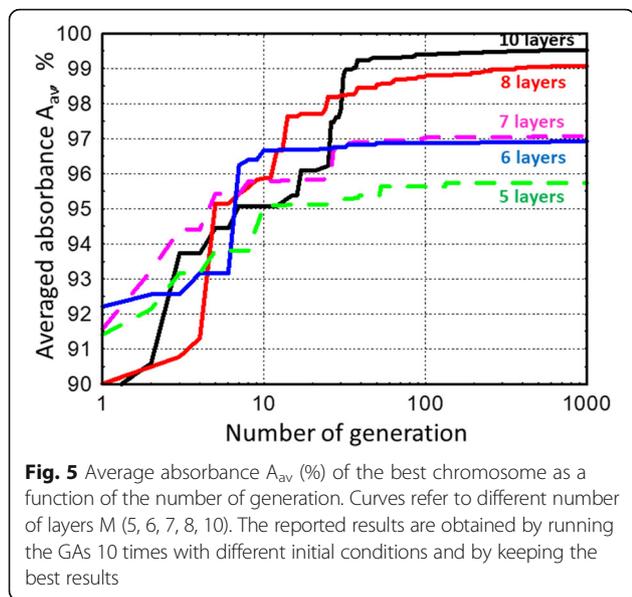
After the selection, N<sub>pop</sub>/2 = 4 couples are formed for reproduction. The reproduction process consists in mixing the genes of each parent couple (X, Y) so to generate the genes of the two sons (S<sub>1</sub>, S<sub>2</sub>) according to the following rule: S<sub>1</sub> = p<sub>1</sub>X + (1-p<sub>1</sub>)Y, and S<sub>2</sub> = p<sub>2</sub>X + (1-p<sub>2</sub>)Y where p<sub>1</sub> and p<sub>2</sub> are weights randomly chosen from 0 to 1. For example in Table 2 the couple of parents N.5 and N.6 generates the couple of sons N.5 and N.6 in Table 3. The first gene of the sons (S<sub>1</sub> = 65, S<sub>2</sub> = 72) (cells are highlighted in black in Table 3) are obtained by mixing the first gene of their parents (X = 49, Y = 89) (cells are highlighted in black in Table 2) by using the weights p<sub>1</sub> = 0.6 and p<sub>2</sub> = 0.42. This procedure is repeated for all the genes by changing randomly p<sub>1</sub> and p<sub>2</sub>. In this example the fitness of the sons (414, 358) is higher than the ones of their parents (74, 63). In general after reproduction a new population of children is generated (see Table 3), which statistically has an average fitness better than the previous one (see Table 2), thanks to the selection rules, and to the general assumption that good parents generate good children. In synthesis the new generation tends to adapt more to the environment. Sometimes it happens that after several generations, the individuals become too similar to each other. This unwanted phenomenon may

produce an evolutionary stop (epistasis) which inhibits further improvement of the population. To avoid the epistasis, a random mechanism of mutation of the genes should be introduced. Accordingly each single gene may be mutated and substituted by a random value (within the appropriate range seen in section 2) but this may happen only with a small probability (probability of mutation is set to P<sub>m</sub> = 5%). This value is given by a tradeoff as shown in a previous work [30]. In fact P<sub>m</sub> < 5% could cause the epistasis, while P<sub>m</sub> > 5% generates random mechanisms for the research of the optimal solution which become dramatically time consuming). This mutation creates a new chromosome, sometimes extremely different from its parents, but anyway useful for the renewal of the population. For example in Table 4, the four genes highlighted in black are mutated



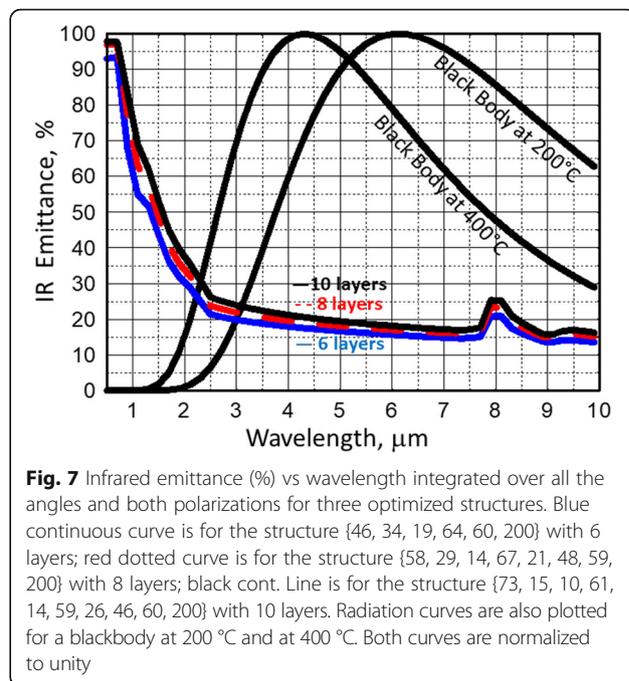
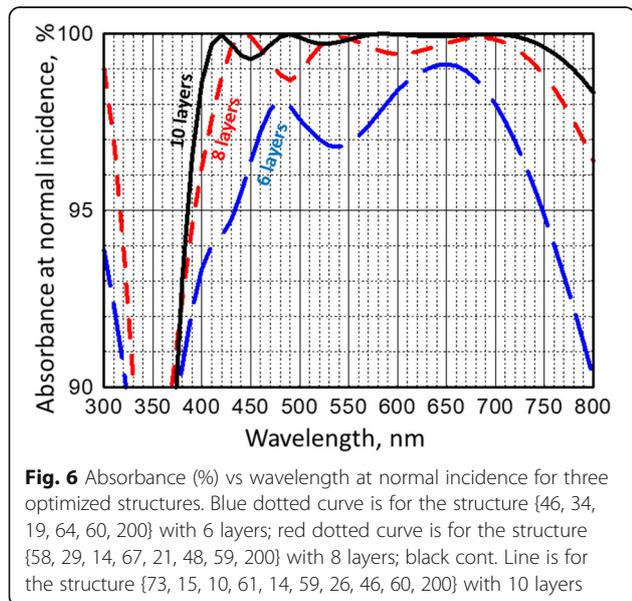
**Fig. 3** Average absorbance A<sub>av</sub> (%) of the best chromosome as a function of the number of generation. Curves refer to different size of the population N<sub>pop</sub> (8, 10, 12, 14). The reported results are obtained by running the GAs 10 times with different initial conditions and by keeping the best results





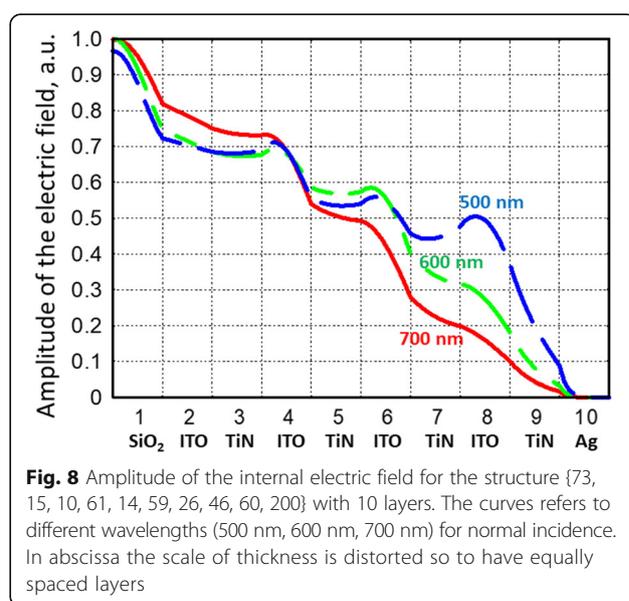
the optimal string {46, 34, 19, 64, 60, 200} also shown in Table 5 (for  $M = 6$ ) where the best multilayer structures, calculated by GAs, are summarized for any  $M$  number of layers.

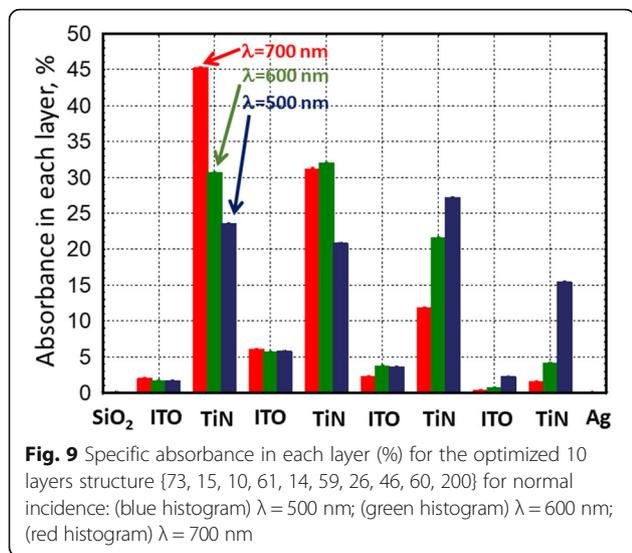
In fact GAs have been also applied to optimize the multilayer structures by changing the number of layers  $M$  (from  $M = 3$  to  $M = 10$ , and according to the scheme in Fig. 2). Figure 5 shows the results of the GAs evolution to optimize the average absorbance  $A_{av}$ . The curves refer to several values of  $M$ , keeping fixed  $N_{pop} = 12$ . All curves saturate after several hundreds of generations tending asymptotically to the optimized multilayer structures reported in Table 5. In principle the maximum achievable absorbance  $A_{av}$  should increase with the



number of layers  $M$ , but with some exceptions. In fact the best performances are obtained when  $M$  is even, when a top silica layer is introduced as an efficient  $\lambda/4$  antireflection coating. This explains why the optimized structure for  $M = 8$  is better than the one for  $M = 9$ , and why the one for  $M = 6$  is almost equivalent to the one for  $M = 7$ .

The absorbance spectra at normal incidence are shown in Fig. 6 only for  $M = 6, 8$ , and 10. The corresponding optimized structures are {46, 34, 19, 64, 60, 200} ( $M = 6$ ), {58, 29, 14, 67, 21, 48, 59, 200} ( $M = 8$ ), and {73, 15, 10,





61, 14, 59, 26, 46, 60, 200} ( $M = 10$ ), reaching a very high average absorbance  $A_{av}$  of 96.9%, 99.1% and 99.5% respectively.

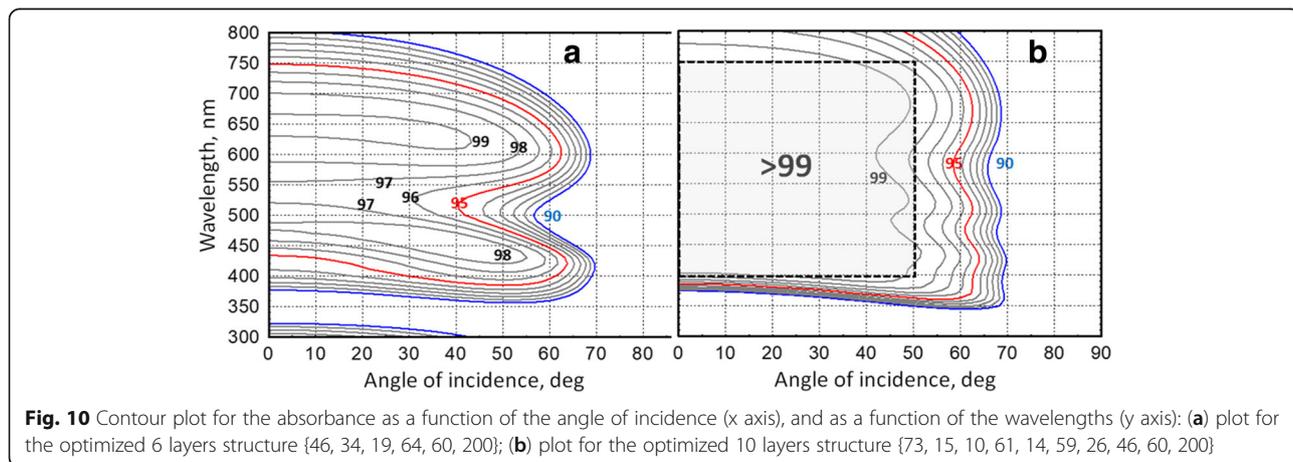
In order to evaluate the infrared properties of these three optimal structures, we calculate the emissivity spectra from  $0.5 \mu\text{m}$  to  $10 \mu\text{m}$ , integrated for all angles and averaged for both polarizations (see Fig. 7). By a first inspection of Fig. 7 the emissivity drops in the infrared range for all the curves. Finally the hemispherical total emissivity has been also evaluated at two different temperatures ( $200^\circ\text{C}$  and  $400^\circ\text{C}$ ) representing the typical thermodynamic range of most solar collectors. In practice the hemispherical total emissivity at  $200^\circ\text{C}$  and at  $400^\circ\text{C}$  are calculated by integrating, over the whole spectrum, the emissivity spectra weighted by the black body radiation curves at  $200^\circ\text{C}$  and at  $400^\circ\text{C}$  that are shown in Fig. 7 in normalized scale. The values of the hemispherical total emissivity  $\epsilon_{IR}$  at  $200^\circ\text{C}$  and at  $400^\circ\text{C}$  are reported in Table 5 for all the structures. The quantity

$\epsilon_{IR}$  slightly increases with the number of layers and with temperature, always satisfying the requirement  $\epsilon_{IR} < 20\%$ .

To better understand the absorbing properties of the best optimized multilayer obtained with  $M = 10$ , it is useful to study the internal electric field  $E$  in the whole structure. Figure 8 shows the amplitude of the  $E$  field in each layer at normal incidence. For a better clarity in abscissa the scale of thickness is amplified so to have equally spaced layers. Looking at Fig. 8 an efficient mechanism of distributed absorption is seen at the two wavelengths of  $600$  nm and  $700$  nm. Light penetrates without relevant reflection through the structures, being absorbed by the TiN layers and eventually by the silver layer. Conversely the absorption mechanism at  $500$  nm is related to the light trapping and quasi-resonant absorption [77].

The evidence of the different absorption mechanisms is given by showing the absorbance in each layer along the thin film stack. It is calculated from the difference between the incoming and outgoing Poynting vectors in each layer. Figure 9 show the distribution of the absorbance for the optimized structure with  $M = 10$  {73, 15, 10, 61, 14, 59, 26, 46, 60, 200}, for normal incidence, at  $\lambda = 500$  nm (blue histogram),  $\lambda = 600$  nm (green histogram), and  $\lambda = 700$  nm (red histogram). The absorption occurs prevalently in the TiN layers, but with some differences: at  $700$  nm the light is absorbed in the first TiN layers, while at  $500$  nm, the absorption is enhanced in the internal layers due to a resonance process.

To better analyse the absorbing properties of the structures the contour plots in Fig. 10 represent a useful tool to put together both the wavelength and angular behaviour of the absorbance for two optimized multilayers: for  $M = 6$  layers (Fig. 10a) and for  $M = 10$  layers (Fig. 10b). By comparing the two plots the optimized structure with  $M = 10$  layers obviously shows the best performances in the dotted rectangular area for angles in the range  $[0^\circ - 50^\circ]$  and for wavelengths in the visible range  $[400 \text{ nm} - 750 \text{ nm}]$  which guarantees a huge average



absorbance of 99.5% inside the rectangle. However the results for  $M = 6$  layers are also interesting, showing  $A_{av} \approx 97\%$  but by using a smaller number of layers. In other words the performance increases with the number of layers (see Table 5), and it is understandable that the best sustainable practical solution should be always given by a trade off between the required performance and the structure complexity. It is also worth noting that all structures show a low hemispherical total emissivity till 400 °C (< 20%), fulfilling the requirement for the efficient solar heat collectors.

## Conclusions

The design of quasi perfect absorbers based on ITO/TiN multilayered structures is here discussed. The practical purpose is to find new optimized coatings for solar thermal collectors with the highest achievable absorbance in the visible range from 400 nm to 750 nm, working for a wide range of angles of incidence from 0° to 50°, for both polarizations, and with a low hemispherical total emissivity, so to minimize the radiative losses. Genetic Algorithms are introduced and adjusted for searching the optimal thicknesses for several ITO/TiN multilayered structures with 6, 8, 10 layers reaching a very high average absorbance of 97%, 99% and 99.5% respectively and a low hemispherical total emissivity (< 20%) from 200 °C till 400 °C. The proposed multilayer structures use materials with high thermal stability, and high melting temperature, can be fabricated with simple thin film deposition techniques, appearing to have very promising applications in solar thermal energy harvesting.

## Abbreviations

$A_{av}$ : Absorbance averaged in the wavelength range 400 nm – 750 nm, and in the angular range from 0° to 50°;  $A_0$ : Absorbance for normal incidence averaged in the wavelength range 400 nm – 750 nm;  $\epsilon_R$ : hemispherical total emissivity;  $f$ : Fitness function of the Genetic Algorithms; GAs: Genetic Algorithms; ITO: Indium Tin Oxide;  $M$ : Number of layers of the structure;  $N_{pop}$ : Size of the population of the Genetic Algorithms;  $P_m$ : Probability of mutation;  $SiO_2$ : silica; TiN: Titanium Nitride

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## Availability of data and materials

The numerical results and data can be reproduced by applying the optical method in Ref. [71], by using the Genetic Algorithms described in Ref. [60], and by taking the optical properties of the materials found in Refs. [47, 61–64]. No additional supporting information or data are necessary.

## Author's contributions

The author read and approved the final manuscript.

## Author's information

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## Competing interests

The author declares that he has no competing interests.

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