New metamaterial as a broadband absorber of sunlight with extremely high absorption efficiency

Cite as: AIP Advances 10, 035209 (2020); https://doi.org/10.1063/1.5131630
Submitted: 14 October 2019 . Accepted: 21 January 2020 . Published Online: 06 March 2020

Hussein Akafzade, and Suresh C. Sharma

AVS Quantum Science

Co-Published by

AIP Publishing

RECEIVE THE LATEST UPDATES

© 2020 Author(s).
New metamaterial as a broadband absorber of sunlight with extremely high absorption efficiency

Cite as: AIP Advances 10, 035209 (2020); doi: 10.1063/1.5131630
Submitted: 14 October 2019 • Accepted: 21 January 2020 •
Published Online: 6 March 2020

Hussein Akafzade and Suresh C. Sharma

AFFILIATIONS
Department of Physics, University of Texas at Arlington, Arlington, Texas 76019, USA

Author to whom correspondence should be addressed: sharma@uta.edu

ABSTRACT
We present computer simulations on the design and performance of a broadband and extremely highly efficient (∼98%) CMOS-compatible metamaterial nanostructure for solar energy applications. An optimized unit cell of the nanostructure consists of a 300 nm × 300 nm × 100 nm titanium nitride (TiN) base covered with 60 nm thick SiO₂. A 50 nm high TiN disk of 90 nm radius sits over the SiO₂ dielectric. The TiN disk is capped with another disk of HfO₂ of 90 nm radius and 30 nm height into which six Au nanoparticles (NPs) are symmetrically placed. A periodic array of such unit cells of 300 nm periodicity covers an underlying solar panel. We investigate the performance of the absorber as functions of wavelength, angle of incidence, and polarization of incident sunlight by utilizing the COMSOL Multiphysics software. We observe an impressive absorption of approximately 98% for normal incidence and the broadband range of wavelengths from 250 nm to 1100 nm. Additionally, the absorption is almost independent of the polarization of light and remains higher than 90% for a wide range of incidence angles.

© 2020 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). https://doi.org/10.1063/1.5131630

I. INTRODUCTION
Metamaterials that can absorb broadband sunlight with high absorption efficiency without suffering loss in light absorbance for different polarizations and angle of incidence are important for thermophotovoltaic applications. An additional requirement for an ideal thermophotovoltaic absorber is that its performance does not deteriorate at high temperatures. Numerous metamaterial nanostructures have been proposed with absorption efficiencies in the range of approximately 70%–90% for limited bandwidths of the solar spectrum. In recent years, refractory plasmonic metamaterials have emerged as important materials for energy applications. In this regard, titanium nitride (TiN) is an attractive building block for thermophotovoltaic applications because of its high melting point (2930 °C), plasmonic resonance in the visible (VIS)-to-near-infrared (NIR) range, chemical stability, and compatibility with CMOS fabrication. For example, Chirumamilla et al. have studied the feasibility of 3D TiN pillar-based ultra-broadband absorbers for high temperature applications. Through computer simulations, they observed a polarization independent average absorption of 94% over a 300–2300 nm wavelength range for 320 nm diameter and 1500 nm high TiN nanopillars. Similarly, Wang et al. obtained a light absorption of approximately 93% over a 300–900 nm wavelength range by using TiN-nanopatterns/dielectrics/TiN stack metamaterials. In another study, COMSOL Multiphysics computer simulations by Li et al. obtained absorption exceeding 87% with an average integrated absorption of about 95% over the visible range. Liu et al. have performed computer simulations by using the 3D finite-difference time-domain method for a structure composed of a periodic TiN disk array coated with a 220 nm diameter and 50 nm thick TiO₂ disk array patterned on a 50 nm thick SiO₂ film on a 100 nm thick TiN opaque substrate. They observed a solar weighted absorptivity of 93% with 1110 nm spectral bandwidth over the UV-VIS-NIR range. In the present work, we design a new CMOS-compatible metamaterial nanostructure and study its performance as a broadband solar energy absorber by utilizing the COMSOL Multiphysics software. Our metamaterial nanostructure provides an impressive value of 98% for absorption efficiency integrated over the broadband...
wavelength range of the solar spectrum from 250 nm to 1100 nm. To our knowledge, solar absorption by the proposed metamaterial is the highest for a broad range of wavelength from 250 nm to 1100 nm. Additionally, the incorporation of an excellent high-temperature dielectric hafnium-dioxide (HfO$_2$) adds to the functionality of the absorber at high temperatures.

II. COMPUTATIONAL DETAILS AND STRUCTURE OPTIMIZATION

The simulations presented here were obtained by using the finite element method in the COMSOL Multiphysics software. It is general-purpose powerful simulation software for modeling designs, devices, and processes for scientific research, engineering, and manufacturing. We provide a brief description of the relevant information regarding how the simulations were carried out for the present work. A unit cell of one of the metamaterial nanostructures is sketched in Fig. 1. It is composed of a 300 nm × 300 nm × 100 nm TiN base covered with 60-nm thick SiO$_2$. A TiN disk of 90 nm radius and 50 nm height sits over the SiO$_2$ dielectric and is capped with another disk of a high-temperature dielectric (HfO$_2$) of 90 nm radius and 30 nm height. A set of six 10 nm radius Au NPs is implanted symmetrically in the near surface region of HfO$_2$. A periodic array of such unit cells, with a periodicity of 300 nm,
covers the entire surface of the underlying solar panel. The bottom layer of the unit cell (TiN) provides Ohmic contact through which absorbed energy is transmitted to the solar panel. Because of CMOS compatibility and outstanding optical and physical properties, the HfO$_2$ dielectric is of particular interest. For example, its optical transparency over a wide range of wavelengths from 250 nm to 200 nm, high density (9.68 g/cm$^3$), chemical stability, and high melting point (2758 °C) make it an ideal dielectric for high temperature solar absorbers. We have recently observed superior performance of HfO$_2$ as a dielectric for high sensitivity waveguide-coupled surface plasmon resonance sensors. A mesh used for the simulations presented in this work is sketched in Fig. 2. It is a physics controlled extra fine mesh of a free triangular type, in which COMSOL determines the concentration of the elements according to values of the refractive indices and dimensions of the materials. Obviously, the mesh is the smallest unit. Periodic boundary conditions are imposed on the x–z and y–z walls. Light is incident from the top through a designated periodic port. A second port is added at the bottom of the cube to transmit absorbed energy to the underlying solar panel. The radius and height of each one of the top disks (TiN and HfO$_2$) are optimized to yield the highest absorption coefficient. Figure 3 shows the wavelength dependence of the absorption coefficient. Out of all the simulations which yielded an absorption coefficient higher than 90% for wavelengths ranging from 0.25 μm to 1.1 μm, the 90 nm radius disk provides the highest absorption. An absorber nanostructure having the optimized disk, in conjunction with 50 nm high TiN and 30 nm high HfO$_2$, provides the best results. Figure 4 shows changes in absorption for three different values of the height of the TiN disk. Whereas the nanostructure with 60 nm thick TiN yields higher absorption for wavelengths ranging from about 0.3 μm to 0.6 μm, it is the structure with 50 nm thick TiN which performs better for higher wavelengths. As shown in Fig. 5, absorption is sensitive to SiO$_2$ thickness. For these simulations, only the thickness of SiO$_2$ was varied from 50 nm to 70 nm while keeping all other parameters of the structure fixed at the described optimized values of TiN and HfO$_2$.

The structure with 50 nm thick SiO$_2$ provides the highest absorption of up to about 0.5 μm. In the mid-wavelength range from about 0.6 to 0.75, the structure having 70 nm thick SiO$_2$ yields the highest absorption. For longer wavelengths, the structure with 60 nm thick SiO$_2$ yield the highest absorption.

The final optimized metamaterial nanostructure consists of a 300 nm × 300 nm × 100 nm TiN base covered with 60 nm thick SiO$_2$. A 50 nm high and 90 nm radius TiN disk is placed over the...
SiO$_2$ dielectric. The TiN disk is capped with another disk of an HfO$_2$ dielectric. Six Au NPs, each of 10 nm radius, are accommodated symmetrically over the HfO$_2$ disk.

III. RESULTS AND DISCUSSION

The results presented in this section are obtained for the final optimized structure of the absorber. Figure 6 shows absorption for vertical incidence ($\theta = 0$) as a function of wavelength of the solar spectrum for three different configurations of the unit cell: (1) an optimized unit cell, as shown in Fig. 1, having symmetrically arranged six 10 nm radius Au NPs, (2) the same unit cell except the fact that this unit cell contains four, rather than six, Au NPs, and (3) the same unit cell without any Au NPs. In all three cases, it is remarkable that absorption remains higher than 93% for the entire range of the wavelengths from 250 nm to 1100 nm. The upper range of the wavelength is chosen keeping in view the energy bandgap of the silicon solar panel. These data clearly show that doping the unit cell with Au NPs results in a very significant enhancement in absorption at wavelengths ranging from approximately 500 nm to 950 nm. This finding is consistent with the well-established results that the excitation of localized surface plasmon resonance in Au NPs enhances optical properties of materials. However, the wavelength dependence of the relative change in absorption is different from the wavelength dependence of absorption by NPs themselves. It is well-known that absorption by 10 nm Au NPs peaks approximately at around 510 nm and decreases precipitously at higher wavelengths, approaching zero at about 700 nm. In contrast and as seen in Fig. 6, addition of Au NPs to the unit cell enhances absorption in such a manner that the relative change in absorption reaches maximum at a much higher wavelength of approximately 670 nm and continues being significant up to about 900 nm. Although the increase in absorption is due to the addition of the NPs, the process by which absorption is enhanced appears significantly different from simple absorption of light by the NPs. An understanding of the precise nature of the mechanism behind this difference awaits additional research. Figure 7 compares the solar spectrum on Earth, with water absorption bands around 0.75 \( \mu \)m and 0.95 \( \mu \)m, and the absorption by our optimized metamaterial. The absorption by our optimized metamaterial of almost all the visible solar spectra, that is useful for silicon thermophotovoltaics, is impressive; the magnitude of the largest difference is less than approximately 6% around 0.45 \( \mu \)m. Not only does this metamaterial exhibit exceedingly high absorption efficiency (~98% integrated absorption for normal incidence), it also exhibits near-independence from the angle of incidence over a wide range of angles as well as from polarization of sunlight.

Figures 8 and 9 show how the absorption changes as functions of the wavelength of the incident light and the angle of incidence for both \( p \) and \( s \)-polarizations of sunlight. It is remarkable that for both polarizations, the absorption coefficient is predominantly
higher than 95% for wavelengths from 0.3 \( \mu m \) to 1.10 \( \mu m \) and for incident angles from zero (normal incidence) to 60\(^\circ\). At lower angles of incidence (0\(^\circ\)–35\(^\circ\)), there are two narrow bands from about 0.37 \( \mu m \) to 0.47 \( \mu m \) and from about 0.72 \( \mu m \) to 0.76 \( \mu m \), where absorption is only slightly lower but remains higher than 92% or so. For higher angles, absorption is lower within narrow bands: one around 0.7 \( \mu m \) and the other above 1 \( \mu m \). Between 45\(^\circ\) and 60\(^\circ\), absorption decreases but remains above 85% for both polarizations, except for small range of wavelengths shown by blue shadows.

If the orientation of a solar panel (for example, in the case of a solar panel mounted on a spaceship) can be adjusted continuously such that the sunlight falls upon it vertically, the proposed metamaterial will absorb remarkably 98% of the incident visible energy. As discussed, the incorporation of Au NPs into the nanostructure increases absorption by the metamaterial primarily because of the excitation of the localized surface plasmon resonance. In this context, it is interesting to examine the evanescent fields associated with these excitations. Toward this, we show in Figs. 10 and 11 evanescent electric fields present in two metamaterial nanostructures: one without Au NPs and another with Au NPs embedded in the material. In both cases, \( p \)-polarized light of wavelength \( \lambda = 0.500 \mu m \) is incident normally along the z-axis. Both figures show field distributions in the x–z plane of the structures (the plane of incidence). In the absence of Au NPs, the resonant field is concentrated mostly around the edges of the periodic array of TiN disks. The resonant field at the edges of the disk is approximately \( 6 \times 10^6 \) V/m for 1 mW incidence power and decays exponentially from the edge of the disk with a decay length of approximately 0.05 \( \mu m \). Not only does inclusion of the above-described Au NPs enhance absorption, it also modifies the resonant field and its distribution in the nanostructure because of localized surface plasmons around Au NPs.

The data in Fig. 11 clearly show the concentration of the resonant field around Au NPs, as well as enhanced field distributions at and near the edges of the TiN disks. Once again, the
field around the edges of the disk decays exponentially from the edge of the disk with a decay length of approximately 0.025 μm. These fields are the highest at the interface between the metal (for example, TiN) and the dielectric in the nanostructure without Au NPs. As stated, the fields decay exponentially with increasing distance from the interface. When Au NPs are present in the structure, localized surface plasmons are excited at the interface between Au NPs and surrounding the dielectric, and this gives rise to much higher evanescent electric fields, as shown in Fig. 11. This is reinforced by the data shown in Figs. 6 and 11, where the presence of the Au NPs in the structure further enhances absorption of sunlight because of localized surface plasmons at the metal/dielectric interface in the material. Our choice of HfO$_2$ as an excellent high-temperature dielectric for the proposed metamaterial nanostructure, compared to another CMOS compatible dielectric (Si$_3$N$_4$), is supported by the data shown in Fig. 12. Here, we examine the changes in the relative absorption for a structure in which the HfO$_2$ disk is replaced by a Si$_3$N$_4$ disk. We define relative absorption by $RA = \frac{(A_1 - A_2)}{A_2}$, where $A_1$ and $A_2$ are the absorptions by metamaterial structures having HfO$_2$ and Si$_3$N$_4$ disks, respectively. Si$_3$N$_4$ is also an excellent CMOS-compatible dielectric with optical transparency from ultraviolet to infrared (250–900 nm), a relatively large refractive index (1.91 @ $\lambda$ = 632.8 nm), thermal stability, and good insulating properties. It is widely used by the microelectronics industry as oxidation masks, protection and passivation barriers, gate dielectrics, etc., using the procedure outlined above. These data show that the metamaterial structure with the HfO$_2$ disk performs better as an absorber of sunlight for wavelengths from 250 nm to about 600 nm and much better in the near IR range of wavelengths from about 900 nm to 1100 nm. From about 600 nm to about 900 nm, the metamaterial having the Si$_3$N$_4$ disk outperforms the structure with the HfO$_2$ disk.

IV. CONCLUSIONS

In conclusion, we have investigated a new CMOS-compatible metamaterial nanostructure as a potential broadband absorber of the solar spectrum. The proposed nanostructure can be easily fabricated by using the standard semiconductor fabrication technology tools and high-performance materials, namely, SiO$_2$, TiN, HfO$_2$, and Au NPs. The structural parameters of the nanostructure are optimized by using the finite difference method in the COMSOL Multiphysics software. Subsequently, the performance of the optimized absorber is studied through COMSOL simulations as functions of wavelength, angle of incidence, and polarization of the solar spectrum. The absorption is almost independent of the polarization of sunlight. When integrated over the solar spectrum from 250 μm to 1100 μm, the absorption is ≈98%. The absorbed energy can be transferred efficiently to an underlying solar panel through Ohmic contacts at the base of the absorber.

REFERENCES

1. A. Hubarevich, A. Kukhta, H. V. Demir, X. Sun, and H. Wang, Opt. Express 23(8), 9753 (2015).
2. A. Kukhta, A. Hubarevich, H. Wang, X. Sun, and H. Demir, Physics, Chemistry and Applications of Nanostructures: Reviews and Short Notes (World Scientific Publishing Co., 2013), p. 222.
3. Z. Q. Liu, X. L. Liu, S. Huang, P. P. Pan, J. Chen, G. Q. Liu, and G. Gu, ACS Appl. Mater. Interfaces 7(8), 4962 (2015).
4. K. Aydin, V. E. Ferry, R. M. Briggs, and H. A. Atwater, Nat. Commun. 2, 517 (2011).
5. E. Unal, M.Bagmanci, M. Karaaslan, O. Akgol, and C. Sabah, Int. J. Mod. Phys. B 33(25), 1850275 (2018).
6. M. Bagmanci, M. Karaaslan, E. Unal, O. Akgol, M. Bakir, and C. Sabah, Int. J. Mod. Phys. B 33(6), 1950056 (2019).
7. P. Rupangura and C. Sabah, J. Nanophotonics 12(2), 26022 (2018).
8. P. Yu, L. V. Besteiro, Y. J. Huang, J. Wu, L. Fu, H. H. Tan, C. Jagdish, G. P. Wiederrecht, A. O. Govorov, and Z. M. Wang, Adv. Opt. Mater. 7(3), 1800995 (2019).
9. S. Mehrabi, M. H. Rezaei, and A. Zarifkar, J. Opt. Soc. Am. B 36(9), 2602 (2019).
10. Q. Ni, H. Alshehri, Y. Yang, H. Ye, and L. P. Wang, Front Energy 12(1), 185 (2018).
11. S. M. Choudhury, D. Wang, K. Chaudhuri, C. DeVault, A. V. Kildishev, A. Boltasseva, and V. M. Shalaev, Nanophotonics 7(6), 959 (2018).
12. S. Venkataramanabub, G. Nair, P. Deshpande, M. A. Jithin, S. Mohan, and A. Ghosh, Nanotechnology 29(25), 255203 (2018).
13. B. B. Wu and J. G. Wang, Optoelectronic. Adv. Mater.–Rapid Commun. 12(7-8), 417 (2018), see https://oam-rc.inoe.ro/articles/polarization-insensitive-wide-angle-broadband-perfect-absorber-with-patch-structures/fulltext.
14. D. W. Huo, J. W. Zhang, H. Wang, X. X. Ren, C. Wang, H. Su, and H. Zhao, Nanoscale Res. Lett. 12, 465 (2017).
15. D. Y. Jiang and W. M. Yang, Sol. Energy Mater. Sol. Cells 163, 98 (2017).
16. H. C. Wang, Q. Chen, L. Wen, S. C. Song, X. Hu, and G. Q. Xu, Photonics Res. 3(6), 329 (2015).
17. W. Li, U. Guler, N. Kinsey, G. V. Naik, A. Boltasseva, J. G. Guan, V. M. Shalaev, and A. V. Kildishev, Adv. Mater. 26(47), 7959 (2014).
18. P. Patalsas, N. Kalfagianis, and S. Kassavetis, Materials 8(6), 3128 (2015).
19. G. V. Naik, J. L. Schroeder, X. J. Ni, A. V. Kildishev, T. D. Sands, and A. Boltasseva, Opt. Mater. Express 2(4), 478 (2012).
20. Z. Q. Liu, G. Q. Liu, Z. P. Huang, X. S. Liu, and G. L. Fu, Sol. Energy Mater. Sol. Cells 179, 346 (2018).
21. M. Chirumamilla, A. Chirumamilla, Y. Q. Yang, A. S. Roberts, P. K. Kristensen, K. Chaudhuri, A. Boltasseva, D. S. Sutherland, S. I. Bozhevolnyi, and K. Pedersen, Adv. Opt. Mater. 5(22), 1700552 (2017).
22. F. Cao, L. Tang, Y. Li, A. P. Litvinchuk, J. M. Bao, and Z. F. Ren, Sol. Energy Mater. Sol. Cells 160, 12 (2017).
23. COMSOL, https://www.comsol.com/comsol-multiphysics, 2018.
24. K. Tiwari, S. C. Sharma, and N. Hozhabri, AIP Adv. 6(4), 045217 (2016).
25. V. Kolkovsky, K. Lukat, E. Kurth, and C. Kunath, Solid-State Electron. 106, 63 (2015).
26 H. F. Jiao, X. B. Cheng, J. T. Lu, G. H. Bao, Y. L. Liu, B. Ma, P. F. He, and Z. S. Wang, Appl. Opt. 50(9), C309 (2011).
27 C. Adelmann, V. Sriramkumar, S. Van Elshocht, P. Lehnen, T. Conard, and S. Gendt, Appl. Phys. Lett. 91(16), 162902 (2007).
28 P. Lehan, Y. Mao, B. G. Bovard, and H. A. Macleod, Thin Solid Films 203(2), 227 (1991).
29 S. C. Sharma, in Advances in Sensors: Reviews' Book Series, edited by S. Y. Yurish (IFSA Publishing, Barcelona, Spain, 2018), Vol. 5, pp. 25, http://www.sensorsportal.com/HTML/BOOKSTORE/Advances_in_Sensors_Reviews_Vol_5.pdf.
30 A. Hinojosa and S. C. Sharma, Appl. Phys. Lett. 97(8), 081114 (2010).
31 B. Ding, T. C. Gao, Y. Wang, D. H. Waldeck, P. W. Leu, and J. K. Lee, Sol. Energy Mater. Sol. Cells 128, 386 (2014).
32 Q. F. Zhang, E. Uchaker, S. L. Candelaria, and G. Z. Cao, Chem. Soc. Rev. 42(7), 3127 (2013).
33 S. C. Sharma, J. Murphree, and T. Chakraborty, J. Lumin. 128, 1771 (2008).
34 S. C. Sharma, Mater. Sci. Eng., B 168, 5 (2010).
35 K. Tiwari, A. K. Singh, and S. C. Sharma, Appl. Phys. Lett. 101(25), 253103 (2012).
36 D. Wu, C. Liu, Y. M. Liu, Z. H. Xu, Z. Y. Yu, L. Yu, L. Chen, R. Ma, J. Q. N. Zhang, and H. Ye, RSC Adv. 8(38), 21054 (2018).
37 X. F. Liu, Front. Mater. 5, 1 (2018).
38 C. Radder, B. S. Satyanarayana, and C. Radder, Int. J. Renewable Energy Res. 8(3), 1464 (2018).
39 A. Viswanathan and S. Thomas, J. Alloys Compd. 798, 424 (2019).
40 A. I. Zvyagina, A. A. Ezhov, I. N. Meshkov, V. K. Ivanov, K. P. Birin, B. Konig, Y. G. Gorbunova, A. Y. Tsivadze, V. V. Arslanov, and M. A. Kalinina, J. Mater. Chem. C 6(6), 1413 (2018).
41 J. Cao, T. Sun, and K. T. V. Grattan, Sens. Actuators, B 195, 332 (2014).
42 E. Petryayeva and U. J. Krull, Anal. Chim. Acta 706(1), 8 (2011).
43 Y. Q. He, S. P. Liu, L. Kong, and Z. F. Liu, Spectrochim. Acta, Part A 61(13-14), 2861 (2005).
44 K. Tiwari, S. C. Sharma, and N. Hozhabri, J. Appl. Phys. 118(9), 093105 (2015).
45 S. Yoshinaga, Y. Ishikawa, Y. Kawamura, Y. Nakai, and Y. Uraoka, Mater. Sci. Semicond. Process. 90, 54 (2019).
46 J. S. Park, K. H. Kim, M. S. Hwang, X. Zhang, J. M. Lee, J. Kim, K. D. Song, Y. S. No, K. Y. Jeong, I. F. Cahoon, S. K. Kim, and H. G. Park, Nano Lett. 17(12), 7731 (2017).