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TiN-based metasurface absorber for efficient solar energy harvesting

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ABSTRACT

Solar absorber, which is widely used in concentrated solar thermal systems and solar photovoltaics, has attracted great attention in recent years. Concentrated solar irradiation not only saves production costs, but also effectively improves the photothermal conversion efficiency of the system. However, the huge radiative heat flux will cause the system temperature to rise rapidly, which poses significant challenges for designing solar absorbers. Here, a metasurface absorber based on cylinder array structure is proposed for efficient solar energy harvesting, using the high-temperature resistant materials TiN and SiO2. The total solar absorption of the absorber is up to 0.94 at wavelengths of 300–2500 nm. The high absorption performance of the metasurface absorber can be explained as the coupling effect of surface plasmon resonance and Fabry-Pérot resonance, which is confirmed by the electric field distribution. Moreover, the effect of geometric parameters on absorption performance is analyzed. Finally, we discuss the influence of incident angle on the solar absorber. We believe this work could deepen the understanding of coupling resonance mode and guide the design of high-temperature solar absorbers.

1. Introduction

Energy is decisive in constraining global economic development in the coming decades [[1](#page-5-0)]. Recent studies show that fossil energy, which can cause serious environmental problems, still accounts for more than 80% of global energy consumption. In contrast, as a promising renewable energy, solar energy has advantages in large storage capacity and wide distribution. Specifically, photothermal conversion is one of the most direct and effective ways to utilize solar energy. Concentrated photovoltaic systems use geometrical optical properties to converge low-density solar irradiation on a narrow photovoltaic cell, which effectively improves the conversion efficiency of the system [\[2](#page-5-0)–6]. However, the huge radiative heat flux will cause the system temperature to rise rapidly, which poses significant challenges for designing solar absorbers. Moreover, highly concentrated solar irradiation may damage the surface structure of the solar absorber $[7,8]$ $[7,8]$. Therefore, it is of great significance to investigate high-temperature resistant solar absorbers.

Metasurface, which exhibits exotic properties that are not found in nature, has numerous promising applications in imaging, sensing, and solar harvesting [9–[23](#page-5-0)]. Particularly, solar absorbers based on metasurface have attracted significant attention because of their ability to absorb solar irradiation over a wide range of wavelengths. So far, numerous efforts have been devoted to the design of metasurface solar absorbers [24–[44\]](#page-5-0). Charola et al. theoretically proposed and numerically analyzed a metasurface broadband absorber based on Au and Ti [[45\]](#page-6-0). The results show that the absorber can achieve more than 95% broadband absorption between 550 and 651 THz. Heidari et al. designed a novel broadband, polarization-insensitive absorber [\[46](#page-6-0)]. An average absorption of more than 90% was achieved in the visible region. Azad et al. investigated a metasurface solar absorber consisting of eight pairs of gold nanoresonators [[47\]](#page-6-0). Results show that the absorption was greater than 90% in the solar spectrum, and low emissivity was shown in the mid and far-infrared regions. Although all the above-proposed absorbers have good solar energy absorption performance, the research on high-temperature absorbers is highly desired and worth further exploration.

Here, the metasurface solar absorber is investigated, taking advantage of the high-temperature resistance characteristics of TiN and SiO₂. The absorber comprises a TiN substrate, $SiO₂$ layer, TiN layer, and TiN cylinder array. The total solar absorption (AM1.5 data) of the absorber is analyzed. The electric field distribution can reveal the high absorption performance of the metasurface absorber. Moreover, the geometric

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Fig. 1. (a) Schematic diagram of the proposed metasurface absorber. The period, diameter and height of the cylinder array structure are *L*, *D*, and *h*1. The thicknesses of TiN and SiO₂ layer are *h*₂ and *h*₃. The light is incident obliquely from the air at angle of *θ* on the proposed metasurface absorber in the x-z plane. (b) Simple flowchart for the general fabrication procedure of the metasurface absorber.

parameters effect of the solar absorber on absorption performance is analyzed. Finally, we discuss the influence of incident angle on absorption performance for different polarizations.

2. Models and methods

Fig. 1(a) gives a schematic diagram of the proposed metasurface absorber based on the cylinder array. The high melting point materials TiN (2950 °C) and SiO₂ (1723 °C) are used. The absorber comprises a TiN substrate, $SiO₂$ layer, TiN layer and TiN cylinder arrays. Compared to absorbers formed by metallic nanoresonant cavities, TiN-based solar absorbers have greater thermal stability [48–[50\]](#page-6-0). It can not only reduce the cost but also improve the high-temperature resistance of the absorber. The period is $L = 400$ nm. The diameter and height of the cylinder array are $D = 240$ nm, and $h_1 = 150$ nm. The thickness of the TiN layer and $SiO₂$ layer are $h₂ = 5$ nm and $h₃ = 170$ nm. The thickness of the TiN substrate is set as 500 nm to reduce the transmittance. The light is incident obliquely at angle of *θ* in the x-z plane for transverse magnetic (TM) or transverse electric (TE) polarization. Permittivities of TiN and $SiO₂$ can be found in Ref. [[51\]](#page-6-0). The default conditions are the incidence angle $\theta = 0$ and TM polarization unless otherwise specified. Fig. 1(b) gives the general fabrication procedure of the metasurface absorber. First, the TiN substrate is deposited by magnetron sputtering. Followed by ultrasonic cleaning TiN substrate and using an ion beam sputter in the TiN substrate placed $SiO₂$ layer. Then, electron beam evaporation deposits a TiN layer on the $SiO₂$ layer. Finally, microcylinder arrays are fabricated on the TiN layer by UV lithography and reactive ion etching [\[52](#page-6-0),[53\]](#page-6-0).

The spectral absorption performance is calculated by finite difference time domain method. In the simulation, the perfectly matched layer is used as boundary condition in the z-axis direction. For the case where the angle of incidence is 0, we use periodic boundary conditions in the x and y-axis directions. The Bloch boundary conditions are used when the light source is incident obliquely. Power monitors are arranged above the light source and below the absorber to detect reflections and

transmissions. The operating environment of the absorber is air. The spectral absorption *Aλ* and average spectral absorption *Aaverage* are expressed as:

$$
A_{\lambda} = 1 - R_{\lambda} - T_{\lambda} \tag{1}
$$

$$
A_{average} = \frac{\int_{\lambda_1}^{\lambda_2} A_{\lambda} d\lambda}{\int_{\lambda_1}^{\lambda_2} d\lambda}
$$
 (2)

where R_λ and T_λ are spectral reflection and transmission; $\lambda_1 = 300$ nm and λ_2 = 2500 nm are the upper and lower limits of the operating wavelength of the metasurface absorber. Since the thickness of the TiN substrate is large enough, the transmission T_λ is almost 0. The total solar absorption α can be expressed as $[54,55]$ $[54,55]$:

$$
\alpha = \frac{\int_{\lambda_1}^{\lambda_2} A_{\lambda} I_{\text{AM1.5}}(\lambda) d\lambda}{\int_{\lambda_1}^{\lambda_2} I_{\text{AM1.5}}(\lambda) d\lambda} \tag{3}
$$

where $I_{AM1.5}(λ)$ is the spectral intensity of the solar irradiation (AM 1.5 data).

3. Results and discussions

To further highlight the advantages of the proposed metasurface absorber, we exhibit two structures: TiN layer/SiO₂ layer/TiN substrate (Case 1), TiN cylinder array/ $SiO₂$ layer/TiN substrate (Case 2), as shown in [Fig. 2](#page-2-0)(a). It can be seen that the TiN cylinder array (Case 1) and the TiN layer (Case 2) are not used in these two cases, compared to the provided absorber. [Fig. 2\(](#page-2-0)b) shows the spectral absorption of three cases at wavelength of 300–2500 nm. Case 1 has two absorption peaks at wavelengths of 390 nm and 920 nm, both with spectral absorptions above 0.99. These two absorption peaks are attributed to the intrinsic absorption of TiN (390 nm) and Fabry-Pérot resonance (920 nm). Notably, the structure has an absorption valley at wavelength of 600 nm with an absorption of only 0.43 due to the intrinsic loss of TiN. In Case 2,

Fig. 2. (a) Comparison of three different structures of metasurface absorbers: TiN layer/SiO₂ layer/TiN substrate (Case 1), TiN cylinder array/SiO₂ layer/TiN substrate (Case 2), TiN cylinder array/TiN layer/SiO₂ layer/TiN substrate (Proposed absorber). (b) Spectral absorption and (c) spectral solar absorption (AM1.5 data) of three different structures at wavelength of 300–2500 nm.

the high absorption performance is mainly concentrated in the visible band, while the absorption in the near-infrared band is low. The proposed absorber fully uses the structural advantages of these two cases. Compared to Case 1, it effectively overcomes the absorption valley in the visible wavelength band. Compared to Case 2, it enhances the absorption in the near-infrared band. The average spectral absorption of the proposed metasurface absorber is 88.0%, which is 16.0% and 29.9% higher than the other two cases. Fig. 2(c) shows the spectral solar absorption of three cases at wavelength of 300–2500 nm. It can be seen that Case 1 has a large solar radiation loss in the visible band due to the existence of an absorption valley at the wavelength of 600 nm. In addition, for Case 2, the solar radiation in the near-infrared band is not well harvested. Combining the advantages of these two cases, the proposed absorber achieves up to 94.4% of total solar absorption, which is 20.3% and 21.5% higher than the other two cases.

To explain the potential mechanism of the high absorption performance of metasurface absorbers, we calculated the electric field distributions of different structures. [Fig. 3](#page-3-0)(a) and [Fig. 3](#page-3-0)(b) show electric field distributions of Case 1 at wavelengths of 600 nm, and 920 nm. Strong electric field region is concentrated in the air when the wavelength is 600 nm, which proves that the structure has a strong reflection. Therefore, there is an absorption valley at this wavelength caused by the inherent loss of TiN. When the wavelength is 920 nm, the strong electric field is located inside the absorber. The absorption peak can be attributed to the Fabry-Pérot resonance. The electric field in the air is close to 1, proving that the metasurface absorber at that wavelength almost completely absorbs the light. [Fig. 3](#page-3-0) (c) and $3(d)$ give electric field distributions of Case 2 at wavelengths of 600 nm, and 1160 nm. When the wavelength is 600 nm, a strong and symmetrical electric field is excited

at the TiN/air interface above, indicating that the absorption peak can be explained as the combined effect of the intrinsic properties of TiN and surface plasmon resonance. When the wavelength is 1160 nm, the position of the strong electric field region decreases. [Fig. 3\(](#page-3-0)e) and [\(f\)](#page-3-0) show electric field distributions of metasurface absorber at wavelengths of 600 nm, and 1220 nm. Note that the physical mechanism of the metasurface absorber at wavelength of 600 nm is similar to that in [Fig. 3\(](#page-3-0)c). When the wavelength is 1220 nm, the electric field is strongly excited at TiN/air interface as well as in the air. Due to the coupling effect of surface plasmon resonance and Fabry-Pérot resonance, the performance of absorber in the near-infrared region is significantly enhanced.

Moreover, the influence of geometric parameters on absorption performance is investigated. The effect of period *L* is shown in [Fig. 4](#page-4-0)(a). As the increase of period, absorption in the visible region gradually increases, while absorption peak in the near-infrared region possesses blueshifts. It can be seen that the spectral absorption does not fluctuate greatly with the period. As shown in Fig. $4(b)$, the influence of the diameter of cylinder *D* presents an opposite phenomenon. The absorption performance in the visible region decreases, while the absorption peak in the near-infrared region possesses redshifts with increased diameter. The overall absorptive properties also changed little. [Fig. 4\(](#page-4-0)c) shows the influence of the height of cylinder h_1 . The variation of the absorption curve is similar to the influence of diameter *D*. The influence of TiN layer thickness h_2 is shown in [Fig. 4](#page-4-0)(d). When the TiN layer is not used, the absorption spectrum decreases obviously in the near-infrared region. The basic principles are discussed in detail in the previous section. When TiN layer thickness h_2 is not 0, the absorption bandwidth of the proposed metasurface absorber is weakened. One can see that the geometric parameters have little effect on the broadband absorption

Fig. 3. Electric field distributions of Case 1 at wavelengths of (a) 600 nm, (b) 920 nm. Electric field distributions of Case 2 at wavelengths of (c) 600 nm, (d) 1160 nm. Electric field distributions of proposed metasurface absorber at wavelengths of (e) 600 nm, (f) 1220 nm.

Fig. 4. Influence of geometric parameters on the spectral absorption of the proposed metasurface absorber: (a) period *L*, (b) diameter *D* of TiN cylinder, (c) height *h*¹ of TiN cylinder, and (d) thickness h_2 of TiN layer.

Fig. 5. Spectral absorption of proposed absorber versus incident angle for (a) TM, and (b) TE polarization.

performance of the proposed metasurface absorber. This indicates that the absorber has a large manufacturing tolerance, which is conducive to manufacturing the absorber in practical applications.

In practice, solar radiation is mainly divided into TM and TE polarization and the incident angle is uncertain. Therefore, it is essential to consider the effect of incident angle and polarization direction on the absorber performance. Fig. 5 (a) shows spectral absorption varies with the incident angle for TM polarization. It can be seen that the metasurface absorber is highly insensitive to the incident angle. When the incident angle is 60◦, the average spectral absorption can achieve 0.81. Fig. 5 (b) shows the case for TE polarization. The average spectral absorption can be up to 0.68 when the incident angle is 60◦. It can be seen

Fig. 6. Spectral absorption of proposed absorber versus polarization angle for normal incidence.

that the overall absorption characteristics of the absorber exhibit a greater angular insensitivity to TM-polarized light than TE-polarized light in the solar irradiation bands. Moreover, we considered the effect of the polarization angle as shown in Fig. 6. The results show that the proposed metasurface absorber is polarization-independent, which can be explained by the isotropy of the material and the symmetry of the structure.

4. Conclusions

We propose a high-temperature resistant metasurface solar absorber based on TiN cylinder arrays. The average spectral absorption is 0.88, and the total solar absorption is 0.94 at 300–2500 nm. The high absorption performance of the metasurface absorber can be explained as the coupling effect of surface plasmon resonance and Fabry-Pérot resonance, which is determined by analyzing the electric field distribution. The discussion in geometric parameters effect indicates that the absorber has a large manufacturing tolerance, which is conducive to manufacturing the absorber in practical applications. In addition, we find that the proposed absorber still has superior performance (0.81 for TM polarization, 0.68 for TE polarization) at a large incident angle of 60◦. We believe this work will guide us in the design of high-temperature solar absorbers.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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