

Article

Active Broadband Absorber Based on Phase-Change Materials Optimized via Evolutionary Algorithm

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Abstract: This article proposes a temperature-controlled absorber based on VO₂, which consists of five layers: a disk-shaped VO₂ layer array, a dielectric layer, a circular hole VO₂ array, a SiO₂ layer, and a gold substrate from top to bottom. We optimized the thickness of the other four layers of the absorber, except for the gold layer, using PSO. After ten iterations, we determined that the optimal parameters for the top-to-bottom four-layer thicknesses were 0.183 μm, 0.452 μm, 0.557 μm and 1.994 μm. At this point, our absorber reached the optimal absorption parameters, and we plotted the absorption spectrum under these conditions. We found that the absorption rate at 29.1–47.2 THz was higher than 90%, and the absorption bandwidth was as high as 18.1 THz. This frequency band covers most of the atmospheric window area (23–37.5 THz), so it will have good practicality. At 30.8 THz and 43.12 THz, there were perfect absorption peaks with absorption rates of 99.99% and 99.99%, respectively. We explained the cause of absorption from the perspective of electric field, and then we studied the change in the absorption curve of the absorber when the temperature of VO₂ changed, and we can directly observe the changes in the electric field to explain this. Finally, we can tune the bandwidth and absorption rate of the absorber by changing the structure of the VO₂ pattern. After comparing with other absorbers developed in recent years, our absorber still has good competitiveness, and we believe that our solution is expected to have outstanding performance in fields such as photothermal conversion and thermal stealth in the future.

Keywords: VO₂; evolutionary algorithm; broadband absorber; mid-infrared

1. Introduction

A metamaterial is a synthetic material, which means it is not naturally occurring. Because of metamaterial's customizable electromagnetic properties, it can readily exhibit electromagnetic characteristics that natural materials lack, thus greatly expanding the

potential applications of metamaterials [1–6]. In the field of absorbers, the research of Landy's team in 2008 led to the upsurge of applying metamaterials to absorbers [7]. Since then, metamaterial absorbers have been widely used in thermal radiation absorption, optical stealth, intelligent windows and other fields [8–12], while metamaterial narrowband absorbers have outstanding performance in sensor, detection and other fields [13–17].

At present, metamaterials such as Dirac metal, Graphene, and VO₂ are most widely used in metamaterial absorbers [18–22]. This is due to the phase-change characteristics of VO₂ discovered by Bell Labs in 1959 [23], namely that VO₂ is in an insulating state at room temperature, and when it is heated to 340 K, it transitions into a metallic state. Because the phase-change temperature is closer to room temperature than other materials, researchers have always been enthusiastic about VO₂ research. In 2021, Zhong [24] proposed an absorber based on a combination of gold and VO₂ layers. The pattern of the absorber is composed of a cross-shaped array, with a broadband absorption rate of over 90% at 17–26 THz. In 2023, Kwang's [25] team proposed an absorber based on a toroidal VO₂ array. The absorber has three broadband absorption peaks with an absorption bandwidth of more than 2.42 THz and an absorption rate of more than 90% in the terahertz band. So far, the proposed broadband absorber based on VO₂ has an absorption rate of more than 90%, and the absorption bandwidth is mostly within 10 THz, rarely more than 10 THz. The development direction of broadband absorber must aim for a broader absorption bandwidth while maintaining high absorption rates, which is the direction that researchers need to focus on.

Particle swarm optimization (PSO) is a randomized algorithm proposed by James and Russell in 1995. Inspired by the foraging behavior of birds, PSO initializes the algorithm to randomly assign each particle in the search space, and at the same time, it gives each particle an adaptive speed. Particles can remember the best position they have ever been to, and particle are influenced by three factors: the best position it has ever been to, the best global position, and the initial velocity, resulting in a composite acceleration that iterates to the optimal solution [26]. Compared with other optimization algorithms, PSO has the advantages of wide application range, high computing efficiency, and adaptive adjustment of search strategies.

In this article, we propose a double-layer VO₂ absorber based on a circular hole and disk array, and we optimize its parameters with an improved PSO. The results show that in the frequency range of 29.1–47.2 THz, the absorption rate is above 90%, and the total absorption bandwidth is as high as 18.1 THz. When VO₂ transitions from an insulating state to a metallic state, the highest absorption rate of the absorber increases from 10.3% to 99.99%. We explained the reason for this transition from the perspective of an electric field. Furthermore, we discussed the impact of changing structural parameters on the absorber and addressed the effect of changing the incident angle on the absorber toward the end of the article. Our absorbers have good application prospects in fields such as solar energy absorption and stealth coatings.

2. Particle Swarm Optimization

Earlier, we mentioned the basic concept of PSO. We know that the most important thing in PSO is to iterate the position and speed of particles as well as the optimization strategy [27,28]. Although the traditional PSO is convenient to search the optimal solution globally, it takes a long time to search locally, so we chose the improved particle swarm optimization algorithm. The iteration formula of speed and position is as follows [29,30]:

$$newv = wv + c_1 * rand * (gbest - x) + c_2 * rand * (pbest - x) \quad (1)$$

$$newx = x + newv \quad (2)$$

$$w = w_{max} - \frac{d}{maxd} * w_{min} \quad (3)$$

where w is the inertia weight, v and x are the current velocity and position, $newv$ and $newx$ are the updated velocity and position, c_1 and c_2 are acceleration constants, $rand$ is a random number within 1, and $gbest$ and $pbest$ are global and local optimal parameters, respectively. We have defined the weight w that varies with the number of iterations, as shown in Formula (3). We define w_{max} as 0.9 and w_{min} as 0.4. This way, as the iteration progresses, the algorithm switches from searching for global optimal values to searching for local optimal values, greatly enhancing the accuracy and efficiency of the search [31].

In the combination of absorbers and the PSOs in the past, most researchers often choose the average absorption rate of the region as the figure of merit (FOM), which ignores the need for broadband absorbers to meet a wider absorption bandwidth. Therefore, after discussion, we define the formula of FOM as follows [32–34]:

$$FOM = bw_{pre}/bw_{total} \quad (4)$$

where bw_{pre} is the absorption bandwidth with an absorption rate higher than 90%, and bw_{total} is the total bandwidth selected.

Unfortunately, due to the inherent nature of the algorithm, PSO algorithm cannot be well applied in the current hot field of hypersurface inverse design, like random forest (RF) and deep learning (DP). However, in terms of optimization problems, PSO has rare advantages compared to the above two algorithms.

3. Design and Method

As shown in Figure 1a, the absorber we designed has a five-layer structure, consisting of a disk VO₂ array, a Topas layer, a circular hole VO₂ array, a SiO₂ layer, and a gold layer from top to bottom. Among them, the radius of circular VO₂ is $r_1 = 0.5 \mu\text{m}$, the thickness $t_1 = 0.183 \mu\text{m}$, the refractive index of dielectric layer is 2.35 [35,36], the thickness $t_2 = 0.452 \mu\text{m}$, the radius of circular hole VO₂ is $r_2 = 0.29 \mu\text{m}$, the thickness $t_3 = 0.557 \mu\text{m}$, the refractive index of SiO₂ layer is 1.90, the thickness $t_4 = 1.994 \mu\text{m}$, and the dielectric constant of the bottom gold layer is described using the drude model, where the plasma frequency $\omega_p = 1.37 \times 10^{16} \text{ s}^{-1}$, and the damping constant $\gamma = 1.23 \times 10^{14} \text{ s}^{-1}$, with a thickness $t_5 = 0.2 \mu\text{m}$ [37,38]. Due to the difficulty in making the absorber we proposed, we have proposed the following production method: first, we deposit a layer of gold on a silicon wafer as the base, and then we prepare a SiO₂ layer on the gold through chemical vapor deposition. Then, VO₂ thin films are generated through magnetron sputtering, and circular holes are generated through chemical etching. For the top layer of VO₂ disk, due to its small thickness, ion beam etching can be used to generate it.

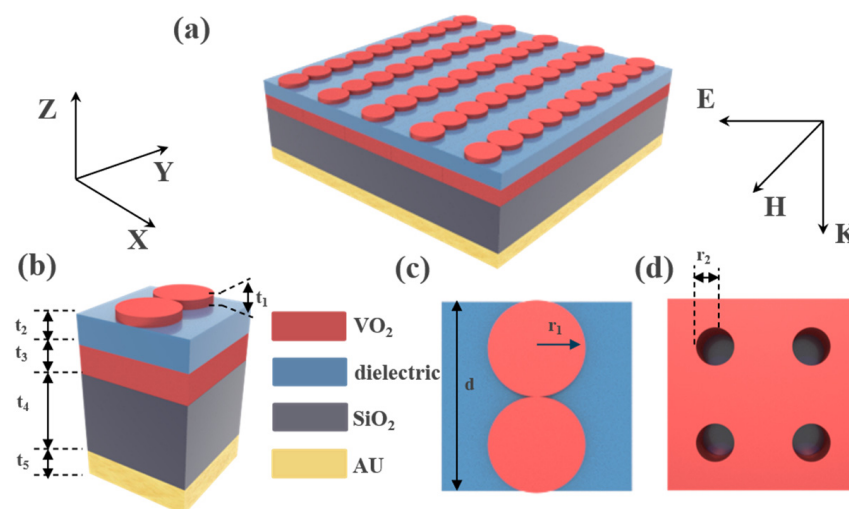


Figure 1. (a) 3D diagram of the array absorber structure; (b) 3D diagram of unit absorber structure; (c) top VO₂ plan view; (d) bottom VO₂ plan view.

The dielectric constant of VO₂ can be described by the following drude model [39,40]:

$$\varepsilon(\omega) = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega(\omega + i\gamma)} \quad (5)$$

where $\varepsilon_{\infty} = 12$, damping frequency $\gamma = 5.75 \times 10^{13}$ rad/s, plasma frequency $\omega_p(\sigma) = \omega_p(\sigma_0)\sqrt{\sigma/\sigma_0}$, where $\omega_p(\sigma_0) = 1.4 \times 10^{15}$ rad/s $\sigma_0 = 3 \times 10^5$ S/m, and without specific instructions, we use the conductivity $\sigma = 2 \times 10^6$ S/m of VO₂ at a temperature of 345 K. We use FDTD Commercial software (Lumerical_2020 R2) for simulation, and the input light wave is the TE wave perpendicular to the absorber surface [41,42]. (See Table 1).

Table 1. Selected parameters and their ranges and minimum accuracy.

Variable	Range (μm)	Minimum Accuracy (μm)
t ₁	0.1–0.3	0.001
t ₂	0.3–0.6	0.001
t ₃	0.5–0.6	0.001
t ₄	1.5–2.5	0.001

The iterative operation of FOM is shown in Figure 2b. When the iteration reaches the tenth time, the optimal solution is obtained. Compared with DP, which requires thousands of training sets and genetic algorithms that require at least fifteen iterations [43], PSO has better speed to achieve the optimal value. The optimal values of the four parameters we obtain are t₁ = 0.183 μm, t₂ = 0.452 μm, t₃ = 0.557 μm, and t₄ = 1.994 μm, respectively. At this point, our absorber reaches its maximum bandwidth above 90%:

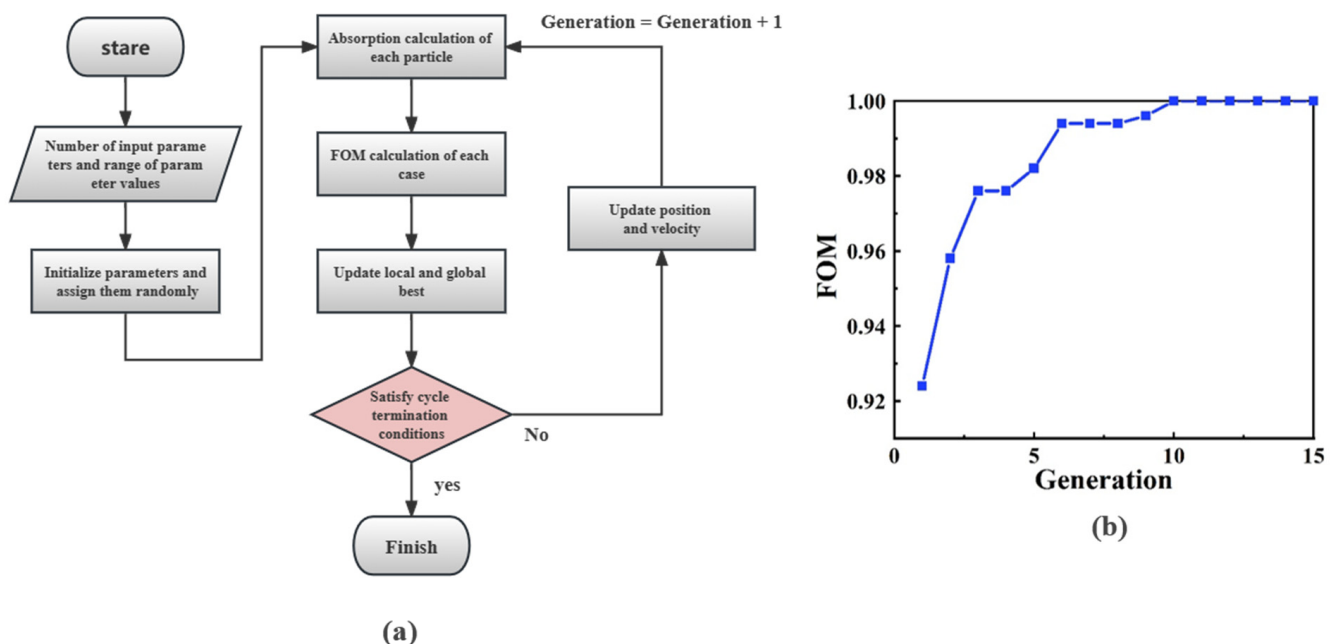


Figure 2. (a) PSO algorithm flowchart; (b) optimizing the FOM process using PSO.

4. Results and Discussions

Figure 3 shows the absorption spectrum of our absorber. The black curve in the figure shows the absorption curve when both the upper and lower layers of VO₂ are present, the orange curve shows the absorption curve when removing the top VO₂, the blue curve shows the absorption curve when removing the bottom VO₂ layer, the green curve shows the absorption curve when removing the upper dielectric layer, and the red curve shows the absorption curve when removing the SiO₂ layer. At this point, we can clearly see that

when we remove any layer structure, the absorption rate can reach up to 97.23%, and the absorption bandwidth above 90% can only reach up to 6.73 terahertz. However, when the five-layer structure is present, the absorption rate can reach up to 99.99%. The absorption bandwidth above 90% is 29.1–47.2 THz, with a maximum of 18.3 THz. The absorption rates at frequencies of 30.74 THz and 43.36 THz reach 99.99% and 99.98%, respectively, achieving perfect absorption. At this time, our absorber has good bandwidth and absorption rate. At the same time, the range of 23–37.5 THz is the atmospheric window, which has a high overlap with our absorption frequency band, which expands the application range of our absorber.

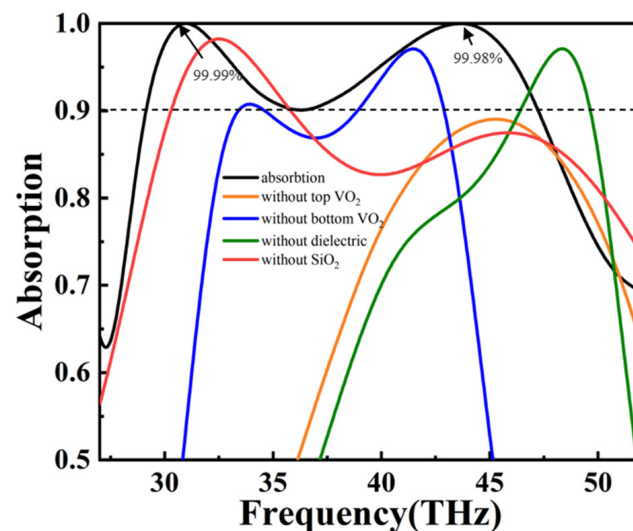


Figure 3. The black curve represents the original absorption curve of the absorber, the orange curve shows the absorption curve when removing the top VO₂ layer, the blue curve shows the absorption curve when removing the bottom VO₂ layer, the green curve shows the absorption curve when removing the upper dielectric layer, and the red curve shows the absorption curve when removing the SiO₂ layer.

In order to explore the reason for the change of absorption rate and absorption bandwidth, we give an explanation from the perspective of electric field.

Figures 4a and 5a show the absorption spectra in the XY direction when both the double layer VO₂ layer and only the top VO₂ layer exist. From these two figures, we can intuitively see that when the bottom VO₂ layer is removed, the intensity of the electric field in the upper layer VO₂ decreases. At the same time, the electric field attached to the x direction of the disk undergoes some dissipation, flowing towards the surrounding medium, resulting in a decrease in absorption [44,45]. Figures 4b–d and 5b–d show the absorption spectra of the bottom VO₂ layer in the XY, XZ, and YZ directions. Figure 4b–d show the absorption spectra when the top VO₂ layer exists, and Figure 5b–d show the absorption spectra when the top VO₂ layer is removed. From Figure 5b–d, we can see that when there is only the bottom VO₂ layer, the electric field undergoes large-scale resonance in the cavity inside the circular hole and the upper layer of the ring. Local surface plasmon resonance occurs at the bottom of the circular hole, and the intensity of the electric field is also low [46,47]. From Figure 4b–d in comparison, we can see from the electric field graph in the XY direction that the large-scale resonance inside the circular hole has disappeared. By observing the electric field patterns in the XZ and YZ directions, we found that surface plasmon resonance appeared in the upper layer of the circular hole, and the overall electric field intensity also increased significantly, enhancing the absorption of light [48,49]. In summary, the presence of double-layer VO₂ enhances the local surface plasmon resonance of VO₂, reduces large-scale resonance, and increases the absorption of light via the absorber, which explains why we use double-layer VO₂.

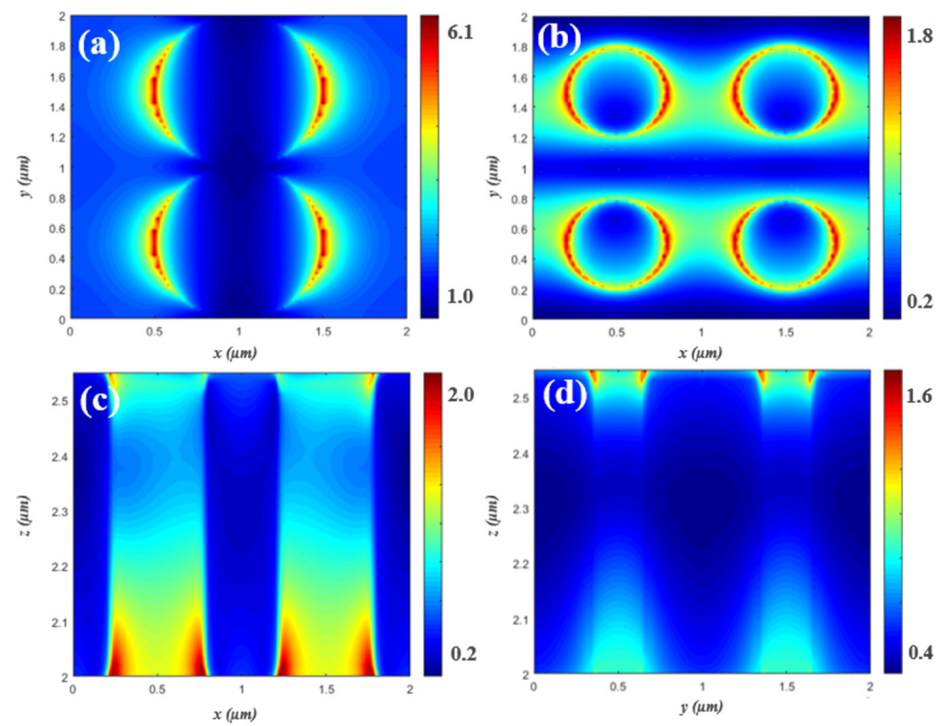


Figure 4. (a) The electric field diagram of the upper VO₂ layer of the absorber we proposed in the XY direction; (b) the electric field diagram of the lower VO₂ layer of the absorber we proposed in the XY direction; (c) the electric field diagram of the lower VO₂ layer of the absorber we proposed in the XZ direction; (d) the electric field diagram of the lower VO₂ layer in the YZ direction of our proposed absorber.

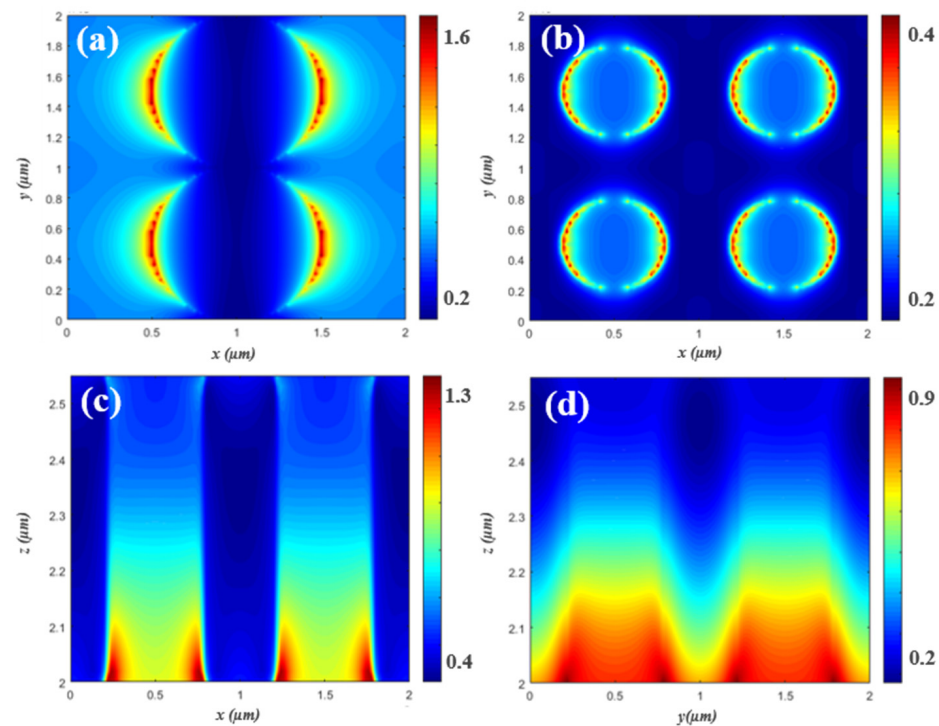


Figure 5. When removing the lower layer VO₂, (a) shows the electric field diagram of the upper layer VO₂ in the XY direction of our proposed absorber; when removing the upper layer VO₂, (b) shows the electric field diagram of the lower layer VO₂ in the XY direction of our proposed absorber; (c) the electric field diagram of the lower VO₂ layer of the absorber we proposed in the XZ direction; (d) the electric field diagram of the lower VO₂ layer in the YZ direction of our proposed absorber.

The specific crystal structure of VO₂ results in its phase transition [50,51]. As shown in Figure 6a, we have plotted the effect of VO₂ at different temperatures on the absorption curve of the absorber under heating. At the same time, we can see the phenomenon of conductivity hysteresis during the heating and cooling processes, which is usually considered to be caused by the combined effect of thermal expansion coefficient and internal stress [52,53]. We found that when VO₂ is at 318 K, which is maintained at a low temperature, the overall absorption rate of the absorber is within 12%. However, when the temperature is heated to 340 K, VO₂ begins to phase change, and the overall absorption rate of the absorber increases, with the highest absorption rate reaching 28.7%. As the temperature further increases, we can see that the absorption bandwidth and overall absorption rate of the absorber are also increasing. At 342 K, the absorption bandwidth with an absorption rate of more than 90% reaches 14 THz, and at 345 K, when the maximum absorption at both ends reaches perfect absorption, the absorption rate is higher than 90%, and the absorption band width reaches 16.9 THz. In conclusion, we can adjust the temperature to make the VO₂ phase change, so as to tune the absorption rate and absorption bandwidth of the absorber, which makes our absorber more flexible in practical applications.

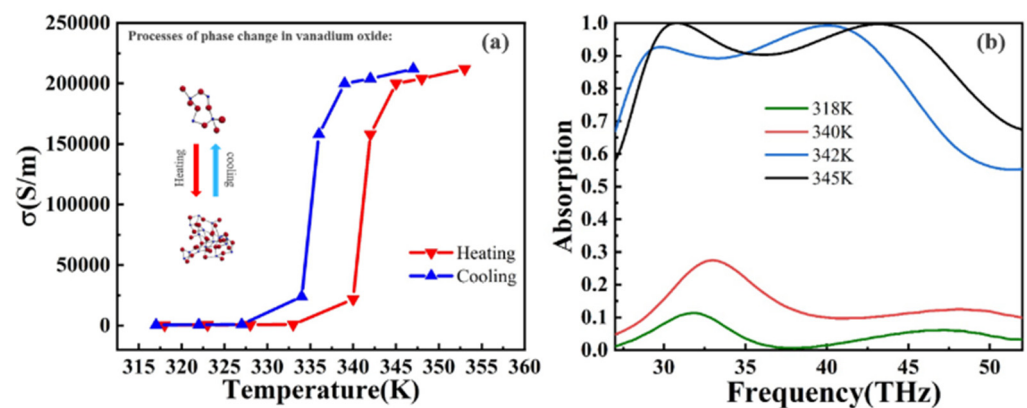


Figure 6. (a) Changes in conductivity of VO₂ with temperature under heating and cooling conditions; (b) absorber absorption spectra at different temperatures.

Similarly, we also studied the electric field diagrams of absorbers under different temperature conditions. As shown in Figures 7 and 8, we have plotted the electric field diagrams of the top and bottom VO₂ layers of the absorber when VO₂ is heated from 318 K to 345 K. We find that when the temperature rises, VO₂ changes from an insulating state to a metallic state, and the electric field intensity of the absorber increases. At the same time, local surface plasmon resonance occurs around the top disc-shaped VO₂ and the bottom circular hole VO₂ inner cavity, which enhances the absorption of light [54–56]. The electric field diagrams in Figures 7 and 8 also prove this.

In order to expand the application field of our absorber, we also conducted research on the structure of the circular hole in VO₂ thin film and VO₂ circular disk. We first studied the radius of the circular hole. With the change in the radius, the absorption curve of the absorber has changed, as shown in Figure 9a. When the circular hole radius is 0.23 μm , the maximum absorption rate of the two peaks from left to right is 30.24 THz and 44.03 THz, respectively, 99.95% and 99.64%. The minimum absorption rate between the two peaks is 88.24%. At this time, the absorption rate at 29.13–35.04 THz and 39.08–47.51 THz is higher than 90%, and the absorption bandwidth is 14.33 THz; When the radius of the circular hole gradually increases to 0.35 μm , the maximum absorptivity of the two peaks from left to right is 30.31 THz and 42.53 THz, 99.99% and 99.53%, respectively, and the minimum absorptivity between the two peaks is 93.04%. At this time, the absorptivity at 29.02–46.24 THz is higher than 90%, and the absorption bandwidth is 17.12 THz. In conclusion, when we adjust the radius of the circular hole from 0.23 μm to 0.35 μm , there is

no significant impact on the absorptivity of the two absorption peaks of the absorber, But the absorption peak on the right has undergone a red shift, and the lowest absorption rate between the two peaks has increased [57,58]. Therefore, we can control the frequency of the absorption peak on the right and the lowest absorption rate of broadband absorption by adjusting the radius of the ring.

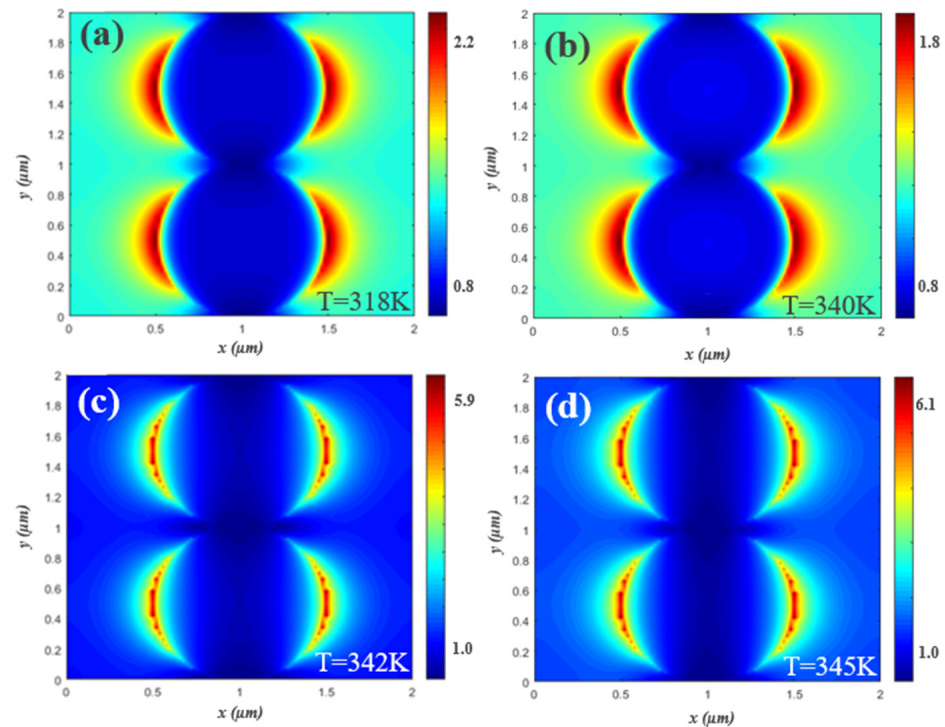


Figure 7. (a–d) Electric field diagrams of VO₂ in the upper layer of the absorber at different temperatures.

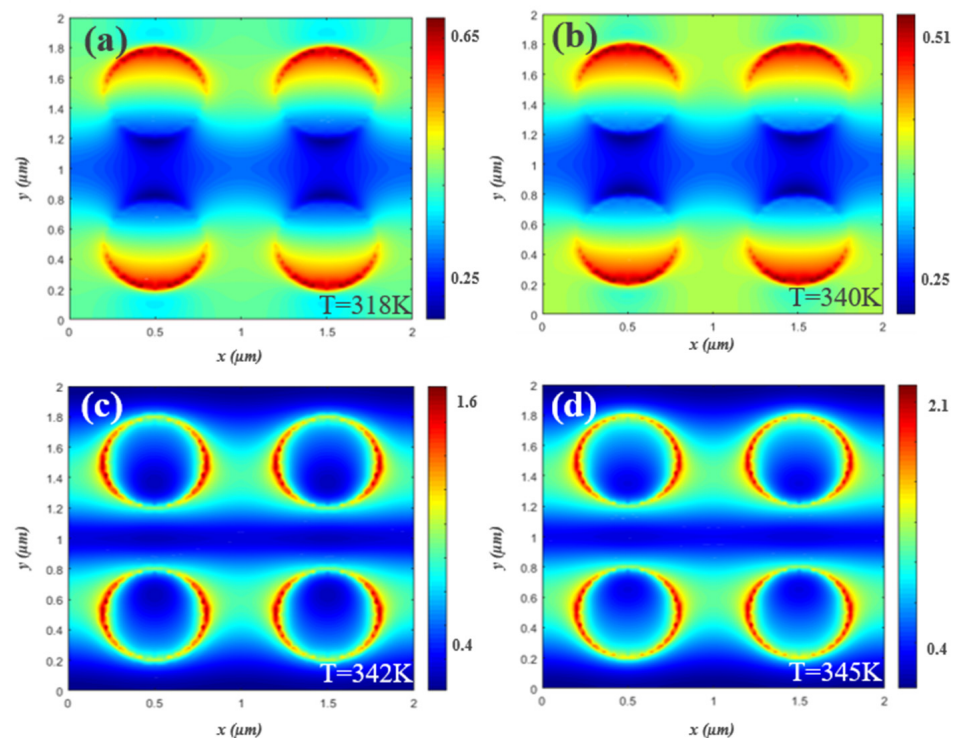


Figure 8. (a–d) Electric field diagrams of VO₂ in the lower layer of the absorber at different temperatures.

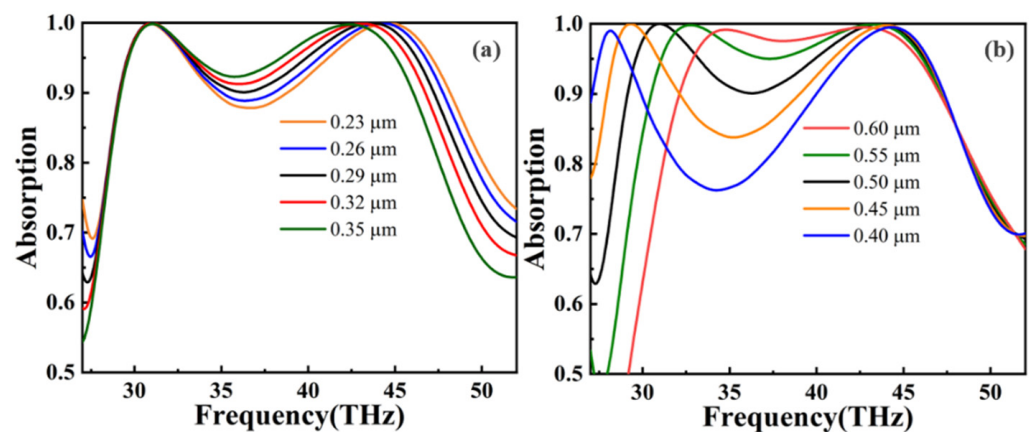


Figure 9. (a) Absorption spectra of VO₂ hole with radius of 0.23, 0.26, 0.29, 0.32, and 0.35 μm ; (b) the absorption spectra of VO₂ disks with radius of 0.60, 0.55, 0.50, 0.45, and 0.40 μm .

Next, we will explore the effect of changing the radius of the disk on the absorber. Figure 9b shows the absorption spectrum when we adjusted the disk radius from 0.6 μm to 0.4 μm . We can intuitively see that as the radius decreases, the left peak of the absorber shifts from 26.12 THz blue to 34.63 THz, the absorption rate increased from 97.54% to 99.99% and then decreased to 98.12%, and the absorption rate of the right peak increases from 98.63% to 99.12%. However, the minimum absorption rate between the two peaks increases from 75.36% to 97.21%, and at a radius of 0.4 μm , the absorption rates at 34.11–44.36 THz are all greater than 97%; that is, the perfect absorption with an absorption bandwidth of 10.25 THz is achieved.

In order to study the practical value and advantages of our absorber, we also discussed the situation at different incidence angles [59,60]. The scanned images of TE and TM waves are shown in Figure 10 and are compared with other absorbers developed in recent years, as shown in Table 2 [61–65]. Figure 10a shows the scanning pattern of TE waves with changes in incident angle. We can see that the absorption curve of the TE wave with an absorption bandwidth of 30–47 THz at an incidence angle of 0–50° has always kept the absorptivity above 80%, and the absorptivity of the two absorption peaks has always been kept above 90%; since our absorber is asymmetric, the TM wave is slightly different from the TE wave, as shown in Figure 10b. When the incident angle is 0–50°, the absorption curve of TM wave is kept above 80% at the absorption bandwidth of 32–49 THz and above 90% at 41–45 THz. In summary, our absorber can still maintain a high absorption rate of over 80% when the incident angle is 0–50°, so it has good practical value [66,67].

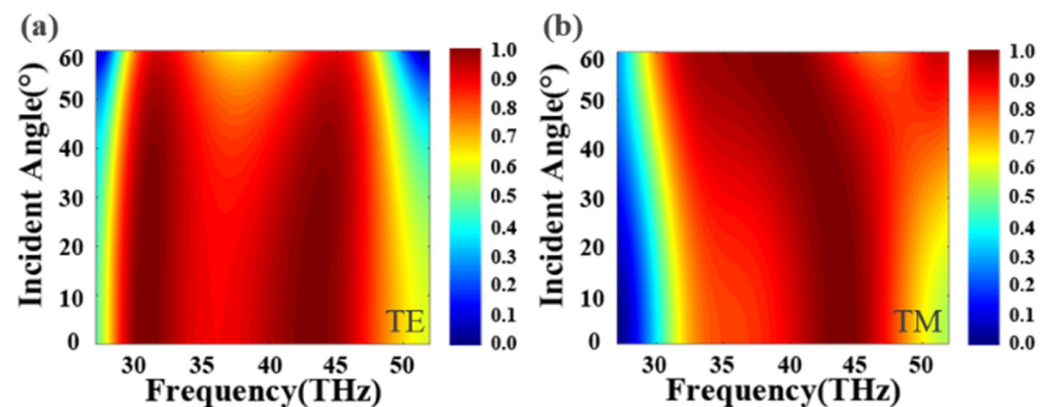


Figure 10. (a) TE wave scanning diagram; (b) TM wave scanning diagram.

Table 2. Comparison of absorbers in this article with other absorbers developed in recent years.

Reference	Operation Band	Max Absoptivity	Structure Layer
[61]	0.4–1.4 THz	96.3%	5
[62]	4.5–9.95 THz	99.9%	5
[63]	4.04–9.41 THz	99.5%	3
[64]	0.52–1.2 THz	98%	6
[65]	11–13 μm	99.9%	3
This work	29.1–47.2 THz	99.99%	5

5. Conclusions

This article proposes a temperature-tunable absorber based on VO₂, which consists of a VO₂ layer, dielectric layer, VO₂ layer, SiO₂ layer, and gold substrate from top to bottom. The top VO₂ layer is an array composed of double-disk patterns, and the bottom VO₂ layer is an array composed of four circular patterns, all of which are simple patterns and easy to process. We applied the PSO algorithm to determine the structure of our absorber and provided an optimization strategy suitable for our absorber, determining the optimal value within ten iterations. We drew the absorption spectrum of the absorber and found that the absorption bandwidth of 29.1–47.2 THz with an absorption rate higher than 90% was up to 18.1 THz, and there were two perfect absorption peaks in this range, with the absorption rates of 99.99% and 99.98%, respectively. Then, we explained the generation of absorption from the perspective of the electric field, and we studied the impact on the absorption curve of the absorber under the change in VO₂ temperature, which can be seen intuitively from the change in the electric field. Finally, we performed the change in absorption bandwidth and absorption rate of the absorber by adjusting the structure of VO₂ at the top and bottom. Through a comparison with other absorbers developed in recent years, we believe that our absorber has advantages in multiple aspects and is expected to deliver outstanding performance in fields such as photothermal absorption and thermal stealth in the future.

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