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Study on Temperature Adjustable Terahertz Metamaterial Absorber Based on Vanadium Dioxide

YUBING ZHANG¹, PINGHUI WU^{1,2,4}, ZIGANG ZHOU¹, XIFANG CHEN¹,
ZAO YI¹, JIAYI ZHU¹, TIANSHENG ZHANG³, AND HUGE JILE³

¹Joint Laboratory for Extreme Conditions Matter Properties, Southwest University of Science and Technology, Mianyang 621010, China

²Fujian Key Laboratory for Advanced Micro-Nano Photonics Technology and Devices, Research Center for Photonic Technology, Quanzhou Normal University, Quanzhou 362000, China

³School of Science, Huzhou University, Huzhou 313000, China

⁴Collaborative Innovation Center for Ultra-Precision Optical Engineering and Applications, Quanzhou Normal University, Quanzhou 362000, China

Corresponding authors: Zao Yi (yizaomy@swust.edu.cn), Jiayi Zhu (jyzhu@swust.edu.cn), and Huge Jile (hgjl@zjhu.edu.cn)

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ABSTRACT In the study of modern optics, the work of terahertz metamaterial absorbers is mostly multi-band perfect absorbers and ultra-wideband perfect absorbers. In contrast, in practical applications, metamaterial absorbers with adjustable resonance frequency or amplitude play an essential role in many forms. Here, we firstly designed an ultra-wideband terahertz metamaterial perfect absorber, achieving over 99% perfect absorption in the 6.6-8.9 THz range. Secondly, based on the absorber, phase change material VO₂ was added to improve the structure, and three tunable terahertz metamaterial absorbers based on VO₂ were designed, respectively realizing broadband movement and conversion between broadband and multi-band. Also, the terahertz absorber with dynamic tuning characteristics can flexibly control the absorption performance, providing an excellent platform for the realization of terahertz filtering, modulation, and so on.

INDEX TERMS Broadband, multiband, active tuned, vanadium dioxide, high quality factor.

I. INTRODUCTION

At present, the use of photoelectric methods to realize the dynamic and controllable characteristics of metamaterials has attracted more and more attention from experts. Vanadium dioxide, like a phase change material, it is well known that the transition from insulation state to metal state can achieve at 340 K temperature [1]–[4]. With the rise of heat, the lattice structure of vanadium dioxide gradually changed from a monoclinic structure to a four-angle structure, and its conductivity increased steadily in the process of temperature rise [5]–[9]. Therefore, based on the above characteristics, vanadium dioxide has been widely used in the development of thermal responsive photonic electronics and thermal equipment [10], [11].

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In recent years, active and tunable absorbers have received more and more attention [12]–[21]. However, some adjustment methods still need to change some conditions for implementation artificially. So how to achieve true active tunability is a significant development direction of metamaterial absorbers now. In 2010, Huang *et al.* made a metal gold/vanadium dioxide gasket/metal gold composite metamaterial to study the mechanism of the light response. They found that the nanostructures, with vanadium dioxide pads, could be used as dynamic light switches for temperature control [22]. In 2012, Katsetal made a nanoscale metamaterial device that used a thin film layer of vanadium dioxide with a loss of dielectric constant much smaller than the incident wavelength on the sapphire substrate to achieve perfect absorption.

Moreover, the light absorption of 99.75% was realized near the nonmetallic-metallic phase transition of vanadium

dioxide itself [23]. In 2015, Kocer *et al.* made a heat-adjustable short-wave infrared resonance absorber by heating the hybrid alloy-vanadium dioxide nanostructure array above the phase transition temperature of vanadium dioxide [24]. In 2017, Zhu *et al.* generated a “bow-tie” type periodic cell structure and connected vanadium dioxide blocks at the feed point of a single structure to make a surface metamaterial efficient absorber. Experimental results indicate that the structure can achieve an adjustable bandwidth of 360 nm in the near-infrared region. In the terahertz frequency region, the conductivity of vanadium dioxide varies by orders of magnitude following a phase transition [25]. In 2019, the sailors designed a terahertz absorber consisting of a circular resonant ring structure with the electromagnetic response to four frequency bands. The terahertz multi-band absorber was designed and simulated by changing the geometric size of the top metal ring pattern, the dielectric thickness of the middle layer, and the conductivity change rate of the photosensitive silicon at the top metal ring [26]. In the same year, Xia *et al.* designed a photonic crystal structure of the doped silicon with absorption effect is designed to achieve wide-band absorption in the 0.29 to 0.31 THz band, and the photonic crystal has a significant effect on the thermo-optic effect, thereby achieving the function of temperature adjustment [27]. In 2019, Wei *et al.* designed a large-angle mid-infrared absorption switch by introducing the phase change material GST [28]. In 2020, Song *et al.* proposed a multi-layer metamaterial with switchable function based on the phase change characteristics of vanadium dioxide. The combination of the two absorption peaks can make the absorption rate in the wide spectral range of 0.393 THz to 0.897 THz more than 90%. In addition, the research group proposed multi-layer vanadium dioxide-based metamaterial with dual functional properties of absorption and polarization conversion, which can convert linear plane waves into their corresponding cross-polarized waves at 2.0-3.0 THz. The frequency is more than 90% efficient [29], [30].

In this paper, an ultra-wideband terahertz metamaterial absorber is proposed, in which the absorption layer is composed of four T-shaped structures, achieving over 99% perfect absorption in the range of 6.6 THz to 8.9 THz. The mechanism of broadband absorption is analyzed by drawing the electric field and current density diagrams at various frequencies. Besides, we introduced a vanadium dioxide, a phase change material based on a broadband metamaterial absorber. In addition, the basic structure is improved, and three arrangements are designed to realize an active tunable terahertz metamaterial absorber. Its three structures are VO₂-silica-gold-VO₂-silica-gold, gold-silica-VO₂-silica, gold-silica-VO₂-gold. Also, it is proved by simulation that the three structures above can make the absorption bandwidth of the original absorber rise and fall, transfer, and transform the super-bandwidth absorption into multi-band absorption. This actively tunable terahertz metamaterial absorber plays a vital role in many practical applications.

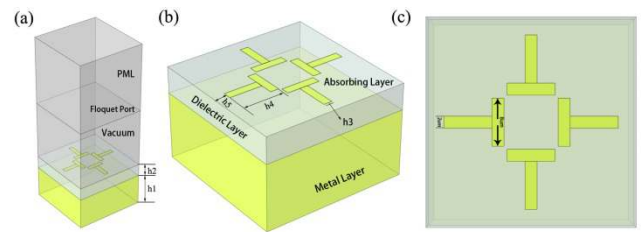


FIGURE 1. Schematic diagram of the base absorber : (a) one unit structure of the absorber, (b) main components of the absorber, and (c) schematic diagram of the absorption layer.

II. DESIGN, SIMULATION, EXPERIMENT, AND THEORY

The model structure of the primary uwb terahertz metamaterial absorber is shown in figure 1. The absorber continues the basic metal-dielectric-metal structure [31]–[35]. In the absorber, the metal materials are all gold, and the conventional silica is selected as the medium material. In the final designed structure, from bottom to top, there are the reflection layer, the medium layer and the absorption layer, with the thickness $h1=16$ μm , $h2=6.34$ μm and $h3=0.05$ μm , respectively, and the period P of the absorber is set as 35 μm . The top of four T-shaped structures, and each T-shaped structure is composed of two rectangles of the same size absorption layer is composed. The length and width of the bases are 8 μm and 2 μm , respectively. The distance between the top of the corresponding T-shaped structure and the bottom of the T-shaped structure is $h4=9$ μm , and the gap between the tail of the T-shaped structure and the bottom of the absorber is $h5=3$ μm . In the selection of material properties, the relevant parameters of gold are represented by the Drude model, and the relative permittivity of silica in the dielectric layer was set as 2.13. We use a finite element method for modeling (COMSOL). We set the boundary conditions of the metamaterial absorber to Floquet. The periodic boundary and the Floquet regular port allow the metamaterial absorber we design to become an infinite array in space. In the process of simulation, the gold at the bottom can well block the incident light, and the transmission (T) of the structure is almost 0 ($T=0$). So absorption can be expressed as $A=1-R$ (reflection) [36]–[40].

In the basic structure, the basic principle is to minimize the reflection coefficient by matching the impedance with the free space and eliminate the transmittance by maximizing the metamaterial loss. The top of the periodic array of metal structure for a metamaterial structure absorbing ability is essential, when the electromagnetic wave incident to metamaterials structure of the upper metal structure, because of its particular geometric parameters and geometry structure, will take place at a particular frequency electromagnetic resonance, based on the Drude model, real ϵ_1 and imaginary part of dielectric constant ϵ_2 can be expressed as [42], [43]:

$$\epsilon_1(\omega) = \epsilon_\infty - \frac{\omega_p^2 \tau^2}{1 + \omega^2 \tau^2} \quad (1)$$

$$\epsilon_2(\omega) = \omega \tau \frac{\omega_p^2 \tau^2}{1 + \omega^2 \tau^2} \quad (2)$$

Angular frequency of the incident electromagnetic wave ω , ω_p is plasma frequency, τ as the relaxation time, ϵ_∞ for Drude constant. When $\omega\tau \gg 1$, a dielectric constant real component can be represented as:

$$\epsilon_1(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2} \tag{3}$$

From the above equation, we can see that as ϵ approaches infinity, the real part of the permittivity is ϵ_∞ . ϵ_∞ reflect the contribution from the polarization of the inner electrons.

In addition to generating resonance, the periodic metal structure array at the top of the infrastructure has another critical function, which is to form impedance matching. By matching the impedance of the structure array with the free space, the reflection of the electromagnetic waves on the surface of the metamaterial absorbing structure can be zero. Such impedance matching can be achieved through specific resonance or plasmon coupling, and metamaterials can be regarded as homogeneous materials at a macroscopic level. The medium layer in the middle of the infrastructure is mainly used to provide space for the electromagnetic wave incident into the absorption structure and absorb the event electromagnetic wave. For ordinary absorbers, to give enough absorption space for electromagnetic waves, materials with relatively sizeable refractive index are generally used to reduce the thickness of the dielectric layer. However, for the absorption structure of metamaterials, the effect of the dielectric layer is not only limited to the absorption of electromagnetic waves but also the electromagnetic resonance satisfying the structure of metamaterials.

In this paper, only the simulation results are considered, and the critical processes for the preparation of the structure are described as follows: (I) liquid phase method or molecular beam epitaxy (MBE) for the preparation of VO₂ films. (II) preparation of gold arrays by electric beam evaporation and ultraviolet (UV) lithography; (III) make dielectric layer 2; (IV) preparation of a VO₂ array by UV lithography and subsequent reactive ion etching.

III. RESULTS AND DISCUSSION

A. ABSORPTION CURVE AND MECHANISM OF INFRASTRUCTURE

Figure 2 shows the absorption curve of the absorber under the foundation structure. We can find in the absorber in 6.5-8.95 THz frequency range you have incredibly high broadband absorption, within the scope of the average absorption can reach more than 98.6%, and 99.9% in many places have high absorption. Compared with other people's work, the absorption bandwidth has been greatly improved, as shown in table 1 [44]–[48]. To this, we combine the absorber in figure 3 electric field, and current density distribution on the absorption mechanism of the absorber are studied.

In figure 3, we give the distribution of electric field and current density at 7, 8, and 9 THz, respectively. In figure 3, it can be known that the reason for broadband absorption is mainly caused by the resonance coupling of four T-shaped structures. However, due to the influence of polarization

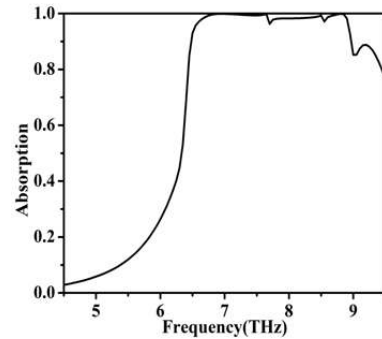


FIGURE 2. The absorption curve of the absorber in the range of 4.5-9.5 THz when the incident angle is 20°.

TABLE 1. Some latest information on VO₂ absorbers.

Refer	type of absorber	Absorption band-width	Modulation depth
[42]	Ultra-broadband THz Absorber	1.63-3.86 THz	Over 90%
[43]	Ultra-broadband near-infrared absorber	1.2-2.5 μm	Over 90%
[44]	Ultra-broadband THz absorber	10.28-15.56 THz	Over 90%
[45]	Dual broadband THz absorber	0.56-1.44 THz and 2.88-3.65 THz	Over 80%
[46]	Broadband THz absorber	1.05-1.6 THz	Over 90%
Present	Ultra-broadband THz Absorber	6.6-8.9 THz	Over 90%

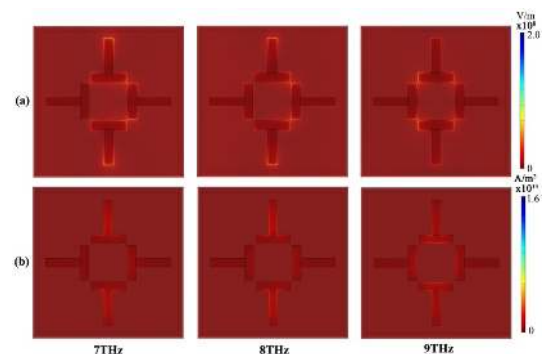


FIGURE 3. (a) and (b) Show the electric field density and surface current distribution of the absorber of 7 THz, 8THz, and 9.00 THz, respectively.

direction, the resonance of two T-shaped structures in the vertical direction is relatively stable and prominent. In contrast, the resonance coupling in the horizontal direction is relatively small. When the electric field at these three frequencies and the current surface diagram are respectively corresponding to the absorption curve, we can better explain the absorption reasons. At 7 and 8 THz, we can find that both the top and the tail of the T-shaped have strong electric fields, while at 9 THz, the generated electric fields mainly exist at the junction of the T-shaped, so the absorption at 9 THz is lower than other places. Also, by observing the current distribution and the pointing vector of the surface current, we can find that the

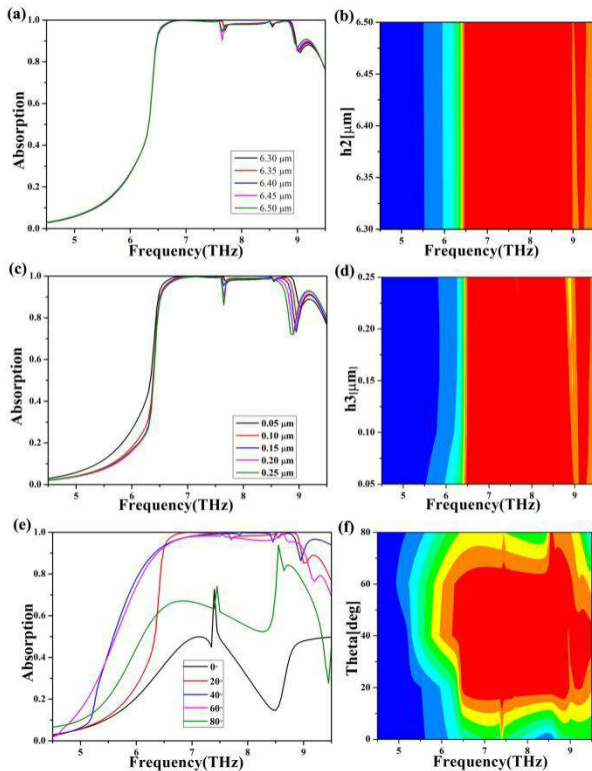


FIGURE 4. The absorption images of the scanning dielectric layer thickness (are shown in (a) and (b)). The absorption images of the scanning absorption layer thickness are shown in (c) and (d). The absorption images of the scanning different angles of incidence (0-80°) are shown in (e) and (f).

current loop can be formed between the four T characters at 7 and 8 THz. In contrast, the current flow at the front end of only T character is steady at 9 THz.

Considering the errors that may occur in the actual manufacturing process of the structure, we continue to analyze the influence of the structural parameters on the resonance. In figure 4, we plot the thickness of the different dielectric layers, the width of the absorbing layer, and the absorption layer when the incident angle is altered. When the thickness of the dielectric layer is changed, the absorption curve has a significant red shift phenomenon. However, when we change the thickness of the absorber dielectric layer in a smaller range, the absorber still has high broadband absorption characteristics, as shown in figure 4 (a) and (b). As can be seen from figure 4 (c) and (d), the absorption value gradually decreases with the increase of the absorption layer thickness. This is because metal materials can support the SPP in visible light, but higher losses and shorter propagation distances will reduce the mass of surface waves. In addition, the absorption rate increases with the increase of incidence angle. This is because as the incident angle increases, the absorption gradually increases. At first, as the reflection of electromagnetic waves increases under high oblique incidence, the absorption decreases with increasing angle. Then, when the incident angle is increased, the magnetic dipole oscillation of the entire absorber is efficiently excited, so that strong absorption

characteristics are maintained at large angles. Generally, the absorber has a good absorption effect on electromagnetic waves with a broader incident angle. Therefore, in the actual structure preparation process, the effects of layer thickness and cell size on the resonance peaks are small.

B. ABSORPTION CURVE AND MECHANISM OF VO₂ ABSORBER

We can use the Drude model to describe the optical dielectric constant of vanadium dioxide in the terahertz band [49]–[53]:

$$\epsilon(\omega) = \epsilon_{\infty} - \frac{\omega_p^2(\sigma)}{\omega^2 + i\gamma\omega} \quad (4)$$

where $\epsilon_{\infty} = 12$ is the relative dielectric constant of vanadium dioxide at high frequencies, $\omega_p^2(\sigma)$ is the conductance dependent plasma frequency, and γ is the damping frequency. In addition, we can see that $\omega_p^2(\sigma)$ and σ are proportional to the carrier density in the free space. Therefore, the plasma frequency can be approximated as an expression.

$$\omega_p^2(\sigma) = \frac{\sigma}{\sigma_0} \omega_p^2(\sigma_0) \quad (5)$$

where $\sigma_0 = 3 \times 10^3 \Omega/\text{cm}$, $\omega_p(\sigma_0) = 1.5 \times 10^{15} \text{ rad/s}$, $\gamma = 5.75 \times 10^{13} \text{ rad/s}$. In the terahertz band, we use parameters such as changing the structural size of the top metal of the absorber to achieve impedance matching between the dielectric layer of the electromagnetic metamaterial absorber and free space. That is, we can adjust the parameters ϵ and μ simultaneously. In this way, we can make them match the impedance $z = \sqrt{\mu/\epsilon}$ of free space. In this way, the reflectance can be reduced in a specific frequency band. When the change of external temperature causes the phase transition of vanadium dioxide, the conductivity of vanadium dioxide changes accordingly, thus breaking the impedance matching with the original structure and the space medium layer, so that the electromagnetic wave is strongly reflected, resulting in the decline of absorption. Similarly, when the temperature conditions remain unchanged, the thickness of vanadium dioxide decreases, and the electromagnetic wave transmission increases, which also leads to the absorption decline. We plot the relationship between conductivity and temperature, as shown in figure 5.

According to the relationship between the dielectric function of the material and the electrical conductivity, we can get the electrical conductivity relationship of the VO₂ film at different temperatures during the phase transition as [54]–[56]:

$$\sigma = -i\epsilon_0\omega(\epsilon_C - 1) \quad (6)$$

Among them, σ is the conductivity of the composite system, ϵ_0 is the dielectric constant of the vacuum, and the dielectric function ϵ_C of the composite system is related to temperature. We offer the relationship between temperature and conductivity, and here we give several corresponding values. At 313 K, the conductivity is 130 S/m; at 333 K, the conductivity is 820 S/m; at 340 K, the conductivity is 21700 S/m; at 342 K, the conductivity is 158000 S/m; at 353 K, the final conductivity is 212000 S/m.

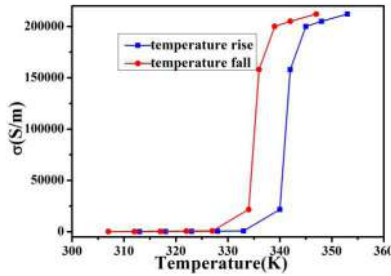


FIGURE 5. Schematic diagram of the relationship between conductivity and temperature.

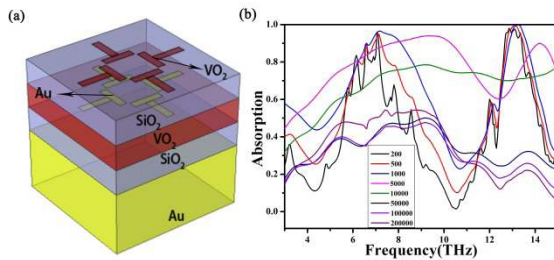


FIGURE 6. (a) Is the main component of structure I type vanadium dioxide metamaterial absorber, (b) is the absorption curve of structure I type vanadium dioxide metamaterial absorber.

C. STRUCTURAL TYPE I VANADIUM DIOXIDE METAMATERIAL ABSORBER

Figure 6 (a) shows that we add two more layers of VO₂ and one layer of SiO₂ to the basic structure. The model of VO₂ terahertz metamaterial active tunable absorber was established. We call it to structure I-vanadium dioxide metamaterial absorber. The structure from top to bottom is a periodic array layer composed of VO₂, a dielectric layer (I), a periodic array layer composed of gold, a VO₂ layer, a dielectric layer (II), and a final layer of Au. To make the absorber have dynamic and adjustable absorption characteristics, we have added two layers of VO₂ to the previously designed primary absorber. One layer is designed for a specific unit structure, and the other layer acts as a dielectric layer. VO₂ can change the internal lattice structure through some effects such as light and heat so that it can be transformed from the insulating phase to the metal phase. In the tunable structure we designed, the conductivity of VO₂ can be controlled by light, so that the temperature change can be controlled. In addition, this structure is equivalent to adding a dielectric layer and an absorption layer, so it is equal to combining two absorbers together. When the temperature of the absorber is higher than the phase transition temperature of VO₂, VO₂ is in the metal phase at this time, and the effect is similar to Au. At this time, it is equivalent to the role of a metal mirror. Light does not pass through this layer structure so that the following structure can be ignored. At this time, the structure only has the top three layers functioning to form an absorber. The active part of the structure is the VO₂ periodic array, the dielectric layer (I), and the VO₂ layer. When the temperature

of the absorber is lower than the phase transition temperature of VO₂, then VO₂ is in the insulating phase. Therefore, VO₂ used in this structure can be considered as a dielectric layer. At this time, the absorbed multilayer structure is similar to the three-layer primary structure in the basic absorber. Therefore, we can control the phase change of VO₂ by adding VO₂ to the central absorber and then realize the active tunable absorption of the absorber.

From the above analysis, we know that temperature affects the conductivity of VO₂, so we draw the absorption curve pattern with the change of conductivity of the absorption under this structure in figure 6 (b). By observing the absorption curve, we can discover that the absorber produces several chaotic absorption peaks when the conductivity is low, and the position of the absorption peak is consistent with that of the infrastructure. However, as the gradual increase of the conductivity, the absorption peak gradually improves. When the conductivity is 500, the absolute absorption peak appears at 2 THz. When the conductivity then rises high enough, we have broadband absorption in the absorber, and broadband is much broader than in the previous infrastructure.

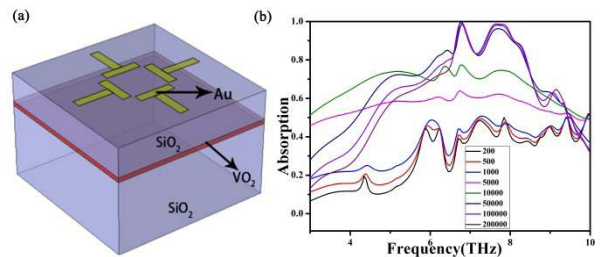


FIGURE 7. (a) Is the main component of structure II type vanadium dioxide metamaterial absorber, (b) is the absorption curve of structure II type vanadium dioxide metamaterial absorber.

D. STRUCTURAL TYPE II VANADIUM DIOXIDE METAMATERIAL ABSORBER

Figure 7 (a) is a schematic diagram of a structural II VO₂ terahertz metamaterial active adjustable absorber. This structure adds a layer of VO₂ to the construction of the original absorber and replaces the metal material at the bottom with a dielectric material. From top to bottom, the periodic array layer-dielectric layer-VO₂ layer-point dielectric layer is composed of gold. When the temperature of VO₂ is low, the structure is equivalent to a metal-dielectric structure and still absorbs part of the incident light. However, since the bottom is made of a dielectric material, projected light is generated. When the temperature of VO₂ rises to the phase transition temperature, the structure is equivalent to a base formed by adding a dielectric layer under the original base structure, and the influence on the absorption curve is not significant.

The absorption curve under this structure is shown in figure 7 (b). We can find that when the temperature is low, the absorption value is shallow due to the presence of transmitted light in this absorber, but it can still be equivalent to

a broadband absorption of 40%-50% at 6-10 THz. As the temperature increases (that is, the conductivity increases), we can see that absorption increases significantly. At conductivity of 10000, there is more than 70% broadband absorption at 4-9 THz. When VO₂ is completely transformed into the metallic phase, it is evident that the structural absorber has an absolute absorption peak and a small broadband generation. Comparing the absorption peak with the frequency of the absorption broadband, we find that the absorption peak is before 6.5-9 THz, which is in perfect agreement with our previous infrastructure.

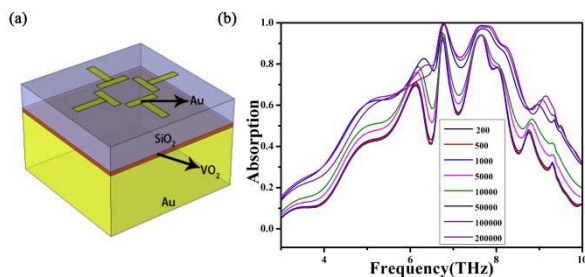


FIGURE 8. (a) Is the main component of structure III type vanadium dioxide metamaterial absorber, (b) is the absorption curve of structure 3 type vanadium dioxide metamaterial absorber.

E. STRUCTURAL TYPE III VANADIUM DIOXIDE METAMATERIAL ABSORBER

Figure 8 (a) is a model diagram of a structural III VO₂ terahertz metamaterial active adjustable absorber. The junction is somewhat similar to structure II, in that it is made up of a layer of VO₂ on top of the original infrastructure, but the material at the bottom is still gold, and the periodic array layer from top to bottom is Au-dielectric layer-VO₂ layer-Au layer. When the temperature of VO₂ is low, the structure is equivalent to a metal-dielectric-metal structure, which is very similar to the basic structure. However, because the relative dielectric constants of VO₂ and SiO₂ are not the same, the dielectric layer formed by the combination of the two is also thicker than the basic structure, so the resonance absorption generated will also be very different from that before. When the temperature of VO₂ rises to the phase transition temperature, the structure is equivalent to that VO₂ forms a reflective metal layer together with gold at the bottom, so the absorption is somewhat similar to that of structure II.

The absorption curve under the absorber is shown in figure 8 (b). We can find that when the electrical conductivity of the absorber is low, the absorber when in the dual-band terahertz metamaterial absorber, but absorption value is not high, the dielectric layer and absorbing layer to produce resonance mode, when the conductivity increased VO₂, absorption curve and structure can be found two absorption curve is similar, this is because at this point, the structure of two and three structure at the top of the absorbing layer and in the middle of the dielectric layer is entirely consistent. The order of the VO₂ with Au layer under the influence on absorp-

tion is not very big, mainly have the effect of absorption of transmitted light.

IV. CONCLUSIONS

To sum up, we firstly designed an ultra-wideband terahertz metamaterial perfect absorber, which achieved over 99% perfect absorption within the range of 6.6-8.9 THz, and mapped the surface electric field and surface current density distribution to study the absorption mechanism. Secondly, based on the absorber, phase change material VO₂ was added to improve the structure, and three tunable terahertz metamaterial absorbers based on VO₂ were designed, respectively realizing broadband movement and conversion between broadband and multi-band. In addition, the terahertz absorber with dynamic tuning characteristics can flexibly control the absorption performance, providing an excellent platform for the realization of terahertz filtering, modulation, and so on.

AUTHOR CONTRIBUTIONS

Conceptualization, Y.Z., P.W., and Z.Y.; data curation, Y.Z., P.W., and X.C.; formal analysis, Z.Y., J.Z., Z.Z., P.W., and T.Z.; methodology, Z.Z., P.W., and T.Z.; resources, P.W.; software, P.W., Z.Z., T.Z., and H.J.; data curation, Y.Z.; writing—original draft preparation, T.Z.; Y.Z. writing—review and editing, Y.Z., P.W., Z.Y., X.C., and J.Z. All authors have read and agreed to the published version of the manuscript.

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(Yubing Zhang and Pinghui Wu contributed equally to this work.)

CONFLICTS OF INTERES

The authors declare no conflicts of interest.

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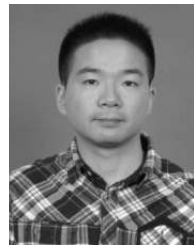
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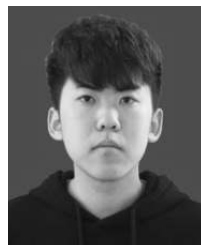
XIFANG CHEN received the B.S. degree from Guangxi Teachers Education University, the M.Sc. degree from Capital Normal University, and the Ph.D. degree in physical from Southeast University, Nanjing, Jiangsu. He is currently a Lecturer with the College of Science, Southwest University of Science and Technology. His research areas are nano luminescent materials and device physics.



ZAO YI received the M.Sc. degree and the Ph.D. degree in condensed matter physics from Central South University, Changsha, Hunan, in 2010 and 2014, respectively. Since 2014, he has been with the Southwest University of Science and Technology, where he is currently a Professor of applied physics. His areas of research interest are plasmonics, nanophotonics, metamaterials, and their applications. He was a recipient of the Doctoral Academic Newcomer Awards of Ministry of Education, in 2012.



JIAYI ZHU received the Ph.D. degree in physical chemistry from the Technical Institute of Physics and Chemistry, CAS, China, in 2014. His research was in the field of self-assembly and optoelectronic property study of graphene-based nanostructured thin films. For two years, he worked as a Postdoctoral Researcher at the Research Center of Laser Fusion, CAEP, where he studied and designed carbon-based ultrablack materials. He is currently an Assistant Professor with the Southwest University of Science and Technology. His current research interests include areas of carbon-based optoelectronic nanostructured thin films and devices and so on.



YUBING ZHANG received the B.S. degree in applied physics from Shijiazhuang University, Shijiazhuang, China, in 2018. He is currently a second-year Graduate Student majoring in physics with the Southwest University of Science and Technology, Mianyang, China. He was admitted to the Physics major of Southwest University of Science and Technology, in 2018. His research interests include the design and manufacture of micro/nano absorbers and terahertz metamaterial absorbers.



PINGHUI WU received the Ph.D. degree in optical engineering from Zhejiang University, China, in 2016. He is currently an Associate Professor with Quanzhou Normal University. His current research interests include the areas of nanophotonics, optical field manipulation and laser physics, and so on.



ZIGANG ZHOU received the Ph.D. degree in science from Suzhou University, in 2005. From July 1999 to July 2005, he worked as a Teacher at Southwest University, where he was engaged in optical teaching and scientific research. In August 2005, he joined the Southwest University of Science and Technology, where he is currently the Associate Dean and in charge of undergraduate teaching, experimental management, and optical teaching. His areas of research

interest are micro-nano optics, integrated photonic devices, optical waveguide passive devices, and laser processing technology.



TIANSHENG ZHANG received the Ph.D. degree in engineering from Gifu University, Japan, in 2012. Since October 2012, she has been a Lecturer with the College of Science, Huzhou University. From May 2016 to April 2017, she worked as a Visiting Scientist at the College of Engineering, Yamagata University, Japan. Her research areas are the synthesis of semiconductor materials and the application in solar cells.



HUGE JILE received the M.S. degree in project management from Hangzhou Dianzi University, China, in 2012. He is currently a Senior Experimentalist with Huzhou University. His current research interests include areas of optical materials, optical design and laser physics, and so on.

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