Switching plasmonic resonance in multi-gap infrared metasurface absorber using vanadium dioxide patches

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Abstract
Reconfigurable metasurface absorbers enable collecting or emitting radiation within selected frequency bands. It is thus necessary to decipher such behavior for many applications, including plasmonic energy harvesting, radiative cooling and thermal emitters. In this article, we propose a compact reconfigurable vanadium dioxide (VO₂)-based metasurface absorber/emitter to demonstrate switching between dual and single-band absorption modes in the mid-infrared regime. The unit cell of the design employs a four-split gold circular ring resonator with gaps filled with VO₂ patches. The phase-transition property of VO₂ between semiconductor and metallic states is used to control the mode of operation of the metasurface absorber. When VO₂ is in the semiconductor state, a dual-band absorption at 6 µm and 10.6 µm is obtained. When it attains a metallic state, the metasurface exhibits a single-band absorption at 8.25 µm. To achieve the maximum absorption efficiency in both single and dual-band modes, adaptive wind-driven optimization was employed as a global optimization technique. The proposed absorber provides polarization-independent behavior for both Transverse Electric and Transverse Magnetic polarizations. Moreover, the proposed design shows above 80% absorptance for incidence angle up to 45° for the dual-band mode, and up to 35° for the single-band mode. When operating the absorber as a tunable emitter, a switching of 79% in emissivity is achieved at 8.25 µm. These favorable findings may facilitate the development of important devices for temperature regulation, smart windows, and thermal imaging.

Keywords: metasurface absorber, vanadium dioxide, phase transition, field confinement, optimization

(Some figures may appear in color only in the online journal)

1. Introduction
Two-dimensional metamaterials are arrays of subwavelength geometries with extraordinary electromagnetic properties that cannot be found in natural materials [1]. These materials are attractive for infrared applications within the atmospheric windows (3–5 µm, 8–14 µm), such as radiative cooling [2], temperature regulation [3], and selective absorption [4]. Metasurfaces promise an alternative to complex optical structures. For example, the inclusion of optimized metasurface absorbers in thermal imaging systems can avoid the use of complex filters and polarizers [5]. The interest in using metasurfaces as electromagnetic absorbers surged following the realization of the first perfect metasurface absorber by Landy et al [6].
Resonant metasurfaces are characterized by very narrowband operation corresponding to the specific geometry of the metasurface. To increase the utility of metasurfaces for wider bandwidths, designing metasurfaces with tunable bandwidth is thus a favorable feature. Active tuning is an effective technique to achieve higher bandwidth [7], provide switching capability [8], and achieve impedance matching conditions [9]. For the GHz range, PIN diodes provide effective switching performance [10, 11]. In the THz range, materials with switchable properties are more suitable as they provide a faster response. Examples include photoconductive materials [12, 13], liquid crystals [14], MEMS [15], and graphene [16].

In the infrared regime, phase transition materials (PTMs) that operate in either a metallic or a semiconductor state are used to tune the response of the metasurface absorber by applying external stimulus such as an electric field [17], current [18], or temperature [19]. Examples of widely used PTMs are vanadium dioxide (VO$_2$) and germanium antimony telluride [3]. VO$_2$ changes from a semiconductor to a metallic phase around a temperature of 67 °C [20]. The employment of VO$_2$ to obtain a tunable absorber was demonstrated for the GHz [21] and THz [22] regimes. Examples include a thin film of VO$_2$ [23] to switch a gold-based absorber between transparency and opacity in the range between 0.2 and 2 THz by heating the VO$_2$ film up to 375 K. Another design was introduced for the same operating range in [24] that provides an ON/OFF ratio of 45 by applying bias voltage to gold electrodes. For these ranges, a simple conductivity variable is used to model the effect of phase transition. This modeling is not adequate to model the phase transition behavior in the infrared regime, and so frequency-dependent complex permittivity models should be employed [25].

In the mid-infrared range, using VO$_2$ as a spacer between a gold antenna and a back reflector was demonstrated in [26]. Results show 3.5% tuning of the resonance frequency and 30% modulation depth around 25.5 THz. A subwavelength thin layer of VO$_2$ deposited over a sapphire substrate achieved a modulation between 0.25% and 80% reflectance using a heating stage between 297 K and 360 K [27]. In [28], a defect engineering was employed to construct a checker-board pattern of VO$_2$. Near zero reflection was achieved at 11.3 µm. The inclusion of VO$_2$ within the gaps of a plasmonic metasurface absorber is an effective way to control the resonance behavior. Examples include placing VO$_2$ patches in the feed gap of gold bowtie nanoantennas [29], and placing VO$_2$ strips in the central gap of aluminum-based absorbers [30]. The results show that the resonance behavior can be modified by changing the current paths within the structure due to the phase transition. In addition, the inclusion of VO$_2$ patches can be used to design multifunctional structures. For example, the phase transition of VO$_2$ was used in [31] to switch the metasurface between perfect absorber operation and operating as a polarization converter. Another example can be found in [32] where VO$_2$ patches are used to switch a metasurface structure between broadband near-perfect absorption and broadband transparency. A dual-to-single band absorber was demonstrated in [2] where VO$_2$ thin film is used to switch the dual absorbance within the atmospheric windows to single absorbance within a non-atmospheric window.

In this work, we propose a compact switchable, polarization-insensitive mid-infrared metasurface absorber that operates in single or dual-band modes by employing the phase-transition property of VO$_2$. The design achieves dual-band absorption at room temperature using a single patterned resonator structured by combining a circular resonator with an inner crossing instead of using two separate resonators for the two bands, thus making the fabrication process easier. In addition, when the absorber operates in dual mode, the absorbed field is highly confined within the VO$_2$ patches embedded in the gaps of a gold resonator. This provides hot spots for energy collection that can be useful for numerous applications such as energy harvesting, sensing, optical trapping, and photocatalysis [33]. Moreover, according to Kirchhoff’s law of thermal radiation, the emissivity of a structure can be deduced from its absorptivity. The proposed structure can thus be operated as a tunable thermal emitter. Our proposed structure achieves switching similar to that reported in [2] using an eight times smaller unit cell; due to the utilization of plasmonic high field enhancement within gaps in addition to interaction between neighboring cells.

2. Structure of absorber

We introduce a single-structured gold resonator that combines the circular ring proposed in [34] with the inner crossing proposed in [35] to support dual-band absorption without using multiple resonators. This simplifies not only the structure but also reduces the fabrication steps [36]. The proposed gold resonator includes symmetrically-placed gaps to provide regions for electric field confinement, which can be useful for applications such as energy harvesting [37] and biosensing [35]. Adding VO$_2$ patches within these gaps provides a mean to change this dual-band behavior into a single-band model by simply changing the operating temperature of the structure. Figure 1 shows the geometry of the unit cell of the proposed metasurface absorber consisting of a top gold resonator of thickness $t_m$ embedded with VO$_2$ patches, a dielectric spacer of thickness $t_s$ and a thick bottom gold film. The gold resonator is patterned in the form of a circular ring of radius $r$ and width $w_1$, combined with an inner cross of width $w_2$. The circular ring has four gaps each of width $g$. These gaps are filled with VO$_2$ patches. The periodicity of the unit cell is $P$ along the two dimensions of the metasurface plane. Inclusion of VO$_2$ within the gaps of a plasmonic metasurface absorber is an effective way to control the resonance. The fabrication scheme reported in [29] can be followed to implement our proposed absorber; the deposition of thick gold back reflector followed by deposition of substrate (e.g. barium fluoride) is straightforward. For the resonator, the pattern of VO$_2$ patches can be defined using a lithography technique, followed by sputtering from a VO$_2$ source, then etching. The gold resonator can then be overlaid over the VO$_2$ pattern using lithography, followed by thermal deposition and lift-off. A practical way...
to activate phase transition in VO$_2$ patches is to mount the structure on a temperature controlling stage as illustrated elsewhere [28].

In the infrared range, gold is modeled as a lossy metal with complex dielectric permittivity. This permittivity attains different values based on the operating frequency. In our work, we used the frequency-dependent permittivity model introduced in [38]. The dielectric spacer is modeled as lossless material whose refractive index has very small variation over the considered infrared range such as barium fluoride and calcium fluoride. When the operating temperature goes above the phase transition temperature of VO$_2$, its electrical permittivity profile changes to a metallic behavior. This change in the material properties shifts the resonance frequencies and the absorption profile, thus achieving the sought tunable response. Two permittivity profiles are used to model the electrical permittivity of VO$_2$ at 30 °C and 90 °C, obtained from [25].

### 3. Simulation and optimization

To investigate the absorption behavior of the proposed structure, we employ the finite element modeling (FEM) method implemented in COMSOL MultiPhysics software$^{(39)}$. A normally incident wave impinging upon the structure in the Z-direction. The electric field is polarized in the X-direction and the magnetic field in the Y-direction. The absorption can be calculated as:

$$A = 1 - R - T,$$

where $R = |S_{11}|^2$ and $T = |S_{21}|^2$ are the reflectance and transmittance of the structure, respectively. Since the bottom gold layer blocks the transmission, $T$ can be ignored in the calculation of $A$. The structure of the plasmonic absorber with no VO$_2$ included in the design provides dual-band absorption resonating at 5.32 μm and 10.4 μm as illustrated in [37]. After placing VO$_2$ patches within the gaps, the resonant wavelengths shifts to 6.2 μm and 10.7 μm when the patches are in the semiconductor state with absorptance values of 84.7% and 83.35%, respectively. The single-band absorption resonates at 7.9 μm when the patches are in the metallic state with an absorptance of 96.5% (see figure 2(a)).

As high absorptance at 10.6 μm is of special interest since it encompasses the ambient infrared radiation from Earth’s surface [37]. We thus targeted placing one of the resonant wavelengths of the dual-band mode at this wavelength. In addition, we explored the effect of changing the metasurface parameters to improve the absorptance behavior. To achieve these objectives, we performed an optimization step starting with the parameter values of the geometry without VO$_2$ patches reported in [37] (see the first row in table 1).

![Figure 1. Geometry of the proposed switchable absorber.](image1)

![Figure 2. Simulated absorptance spectra for (a) the non-optimized structure after placing the VO$_2$ patches, and (b) the optimized absorber including VO$_2$ patches, when the operating temperature is lower (blue) and higher (red) than $T_c$.](image2)

To find the optimal values of the absorber parameters, adaptive wind-driven optimization (AWDO) is employed as a global optimization technique with automated selection of algorithm parameters [40]. AWDO is an iterative evolutionary population-based algorithm that is inspired by the motion of air parcels under the influence of natural forces. The candidate that attains the highest air pressure in this population is considered as the global optimum. The two main equations of the algorithm are the velocity update and position update equations [40]:

$$\begin{align*}
\vec{u}_{\text{new}} &= (1 - \alpha)\vec{u}_{\text{cur}} - g\vec{x}_{\text{cur}} + \frac{i - 1}{i} \gamma_T(\vec{x}_{\max} - \vec{x}_{\text{cur}}) \\
&+ \frac{c \cdot \vec{u}_{\text{cur}}}{i} \frac{\text{other - dim}}{i},
\end{align*}$$

(2)

$$\begin{align*}
\vec{x}_{\text{new}} &= \vec{x}_{\text{cur}} + \vec{u}_{\text{new}} \Delta t,
\end{align*}$$

(3)

| $P$ | $r$ | $w_1$ | $w_2$ | $g$ |
|-----|-----|-------|-------|-----|
| Non-optimized geometry (nm) | 2860 | 1100 | 140 | 415 | 70 |
| Optimized geometry (nm)     | 2780 | 1120 | 140 | 420 | 100 |

Table 1. The optimization variables for the proposed metasurface absorber.

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$\alpha, \gamma, \Delta t$: Parameters of the algorithm.

$\vec{u}, \vec{x}$: Velocity and position vectors.

$\Delta t$: Time step starting with the parameter values of the geometry without VO$_2$ patches reported in [37].
where \( \mathbf{u}_{\text{cur}}, \mathbf{u}_{\text{new}} \) are the current and updated velocity vectors.

The vectors \( \mathbf{x}_{\text{cur}}, \mathbf{x}_{\text{new}} \) are the current and updated position vectors, \( \alpha \) is the friction coefficient, \( g \) is the gravitational constant, and \( \gamma \) is the universal gas constant. \( T \) is the temperature, \( \mathbf{x}_{\text{max}} \) is the solution candidate with the highest pressure, \( c \) is the earth rotational constant, \( i \) is the rank of the current parcel among all the solution candidates, and \( \mathbf{u}_{\text{cur}} \) is the velocity component of one of the other dimensions. The algorithm parameters \( \alpha, g, \gamma T, \) and \( c \) are automatically tuned throughout the iterative process using a covariance matrix adaptive evolutionary strategy [41]. In our study, the position vector includes five dimensions \( \mathbf{x} \in \mathbb{R}^5 \) corresponding to the five optimization variables shown in table 1. The thickness of the substrate and the gold resonator are fixed at 280 nm and 50 nm, respectively. The objective function for optimization is defined as \[42\]:

\[
F = - \min \{ 0.9, A_{\text{semi}} \left( 6 \, \mu m \right) \} - \min \{ 0.9, A_{\text{semi}} \left( 10.6 \, \mu m \right) \} - \min \{ 0.9, A_{\text{met}} \left( 8.25 \, \mu m \right) \},
\]

where \( A_{\text{semi}} \) and \( A_{\text{met}} \) are the absorptance values at the semiconductor and metallic phases of VO\(_2\), respectively. This formulation maximizes the peak absorptance at all resonating wavelengths while maintaining a balanced performance at the three peaks by accepting 90% absorptance. After 50 iterations, the final parameter values are obtained (see the second row of table 1).

4. Results and discussion

The optimal parameter values obtained are used to run full-wave FEM simulation of the absorber. Figure 2(b) shows the simulated absorption spectra for the proposed absorber at different operating temperatures. At room temperature, which is lower than the phase transition temperature of VO\(_2\), the structure behaves as a dual-band absorber with the absorptance of 88.5% and 92.85% at 6 \( \mu \)m and 10.6 \( \mu \)m, respectively. The electric field is confined in the dielectric VO\(_2\) gaps. When the operating temperature goes above the phase transition temperature of VO\(_2\), its electrical permittivity profile changes to a metallic behavior. In this case, the structure behaves as a non-gaped resonator with a single resonance at 8.25 \( \mu \)m and absorptance of 89.64%. This means that a dynamic switching between single and dual-band absorption modes can be achieved by applying different operating temperature without modifying the absorber’s geometry. Moreover, the results in this case show that the optimization step has aligned the maximum absorptance of the hot state with the minimum absorptance of the cold state, achieving a difference in emissivity of 79%, which is favorable for tunable thermal emitter applications. By comparing the variables values of table 1 before and after the optimization step, it is observed that the main parameters that affect the optimization process are the metasurface periodicity \( P \) and the gap width \( g \). \( P \) affects the response by changing the spacing between the patterns of the metasurface, thus defining the amount of interaction between neighboring elements. \( g \) controls the capacitive effect and the accumulation of charges, which defines the level of field confinement within the patches. The other parameters \( r, w_1, \) and \( w_2 \) control the lengths of current paths within the structure and so can finely tune the response.

To better understand the physical mechanism of the switchable absorber, we plot the distribution of the electric field in the horizontal plane cutting the middle of the metallic resonator at the resonant wavelengths, as shown in figure 3. We observe high field confinement within the VO\(_2\) patches at 6.0 \( \mu \)m and 10.6 \( \mu \)m when the VO\(_2\) is operating as a semiconductor. This indicates that the proposed absorber efficiently collects the absorbed field at the resonant wavelengths.

When the operating temperature goes above the phase transition of VO\(_2\), the patches attain metallic properties, so the field confinement becomes weaker at 6 \( \mu \)m and 10.6 \( \mu \)m (see figure 4). The patches in this state form new current paths where the whole structure resonates solely at 8.25 \( \mu \)m. It is worth mentioning that the field concentration at this new wavelength is highest around the ring of the resonator instead of within gaps, which highlights the role of mutual coupling between neighboring cells of the metasurface as shown in figure 4(b). Shifting the resonating wavelength to the middle point between the two wavelengths of the dual-band mode helps in blocking the radiation in the highly transparent ambient range and so prevents the overheating of the structure at high temperature.

In practice, we are interested in harvesting the field incident upon the structure from multiple angles. To quantify the oblique incidence response, we studied the performance of the designed absorber at different incident angles. Figure 5 shows the absorptance versus the angle of incidence between 0° and 70° with a step of 10°. For the low temperature case, the absorber maintains a strong absorption of more than 80% at 6 \( \mu \)m for incidence angles up to 50°. For the resonance at 10.6 \( \mu \)m, more than 80% absorptance is maintained up to around 45°. For the high temperature case, the absorber
provides more than 80% absorptance for incidence angles up to 35°. Since the absorbed field is not confined within the VO$_2$ patches at high temperature, the absorption is spread over a larger bandwidth.

Another spectral feature that can be observed in figure 5 is the appearance of an additional peak close to the main resonance peak at 6 µm. A similar feature was reported in previous work involving a dual-band terahertz metasurface absorber [43], and an isotropic split-ring resonator with gaps [44]. The emergence of this feature can be explained using the effective medium approximation of the resonator as demonstrated in [44], where for oblique incidence, the wave vector component parallel to the resonator surface is non-vanishing, and so impedance matching can be satisfied when the effective magnetic permeability is equal to zero. Such condition takes place at non-zero angles of incidence for wavelengths around 6 µm. To elaborate more on the properties of this additional peak, figure 6 shows a vertical cross-section cut along the VO$_2$ gaps of the metasurface structure with the magnetic field distribution plotted when the angle of incidence is 60°. At 5.9 µm, the magnetic field is concentrated around the gaps. This concentration decreases as the wavelength increases till around 6.3 µm, after which the magnetic field accumulates close to the intersection between the circular resonator and the cross-connector, which corresponds to the additional peak observed in figure 5.

Finally, we tested the robustness of our proposed absorber against variations in the optical properties of VO$_2$. A recent study was carried out in [45] to test the effect of variations of optical properties of VO$_2$ on the phase transition process. The results of the study showed that in the range between 2 and 11 µm, the variations of the optical properties of VO$_2$ induced by different deposition techniques and different substrates are minor as compared to the change of properties induced by the phase transition process due to the low optical loss of VO$_2$ within this range at its cold state. We verified this finding by employing models of VO$_2$ extracted by other researchers from experimental measurements [45–47], as shown in figure 7. It is observed that the model employed in [46] shows an almost constant refractive index in the amorphous state, which is based on extrapolation of data extracted in the near-infrared

Figure 5. The absorptance profile at different angles of incidence at (a) 30° C and (b) 90° C.

Figure 6. The magnetic field distribution at low temperature over the vertical plane cut through the VO$_2$ gaps for oblique incidence angle 60° at (a) 5.9 µm, (b) 6.3 µm, and (c) 6.7 µm.

Figure 7. The complex refractive indices (n, k) of VO$_2$ used to verify the robustness of the proposed metasurface structure against model variations.
Table 2. The values of resonant wavelengths and the corresponding absorptance using different refractive index models for VO2.

| Model | [25] | [45] | [46] | [47] |
|-------|------|------|------|------|
| Resonant wavelengths (µm) | 5.96 | 5.9 | 5.8 | 5.75 |
| | 8.25 | 8.1 | 8.2 | 8 |
| | 10.6 | 11 | 10.6 | 10.5 |
| Absorptance at cold state (%) | 88.51 | 94.41 | 92.37 | 91.23 |
| | 10.2 | 12.04 | 10.88 | 10.723 |
| | 92.85 | 84.85 | 93.35 | 92 |
| Absorptance at hot state (%) | 39.26 | 24.4 | 20.48 | 24.42 |
| | 89.54 | 99.84 | 99.83 | 99.47 |
| | 23.84 | 11.54 | 13.72 | 19.36 |

range. The authors of [46] verified the validation of this model using measurements of a Fourier transform infrared spectrometer. Data extrapolation was also adopted in [48] and the results also showed good agreement with measured data. We applied these models on our proposed absorber and recalculated the resonant wavelengths and the corresponding values of absorptance. Table 2 shows our calculations for the resonant wavelengths and the corresponding absorptance values using these models.

We observe only slight variation in the values of the resonant wavelengths, with high quality switching performance for all models. These results verify that the proposed absorber is robust against variations of optical properties of VO2.

5. Conclusion

We demonstrated a temperature-controlled metamaterial absorber whose tunability is based on the incorporation of VO2 patches within the gaps of gold split-ring resonator. The proposed absorber provides the dual absorption using a single resonator formed by combining a circular ring and an inner crossing instead of using a separate resonator for each band. The electrical permittivity of VO2 can be adjusted by changing the operating temperature, resulting in switching the absorption mode between single and double. The numerical results show that the resonance wavelengths change from dual mode at 6 µm and 10.6 µm to single mode at 8.25 µm when the operating temperature varies from 30°C to 90°C. A suggested extension to this work would be to shift the left resonance at 6 µm to a frequency within the atmospheric window between 3 µm and 5 µm. Another improvement is to modify the design to be easier in fabrication due to the challenge of aligning the VO2 patches inside the gaps of the gold resonator. The proposed absorber can be employed in reconfigurable nanophotonic applications such as tunable filters, modulators, and smart windows.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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