

Article

Design and Machine Learning Optimization of a Dynamically Tunable VO₂-Integrated Broadband Metamaterial Absorber for THz

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Abstract

This paper introduces a vanadium dioxide-integrated broadband metamaterial absorber designed for the terahertz frequency range. The simulation results for the proposed structure demonstrate a wide 90% absorption bandwidth of 8.23 THz, corresponding to a fractional bandwidth of 89.5%. By leveraging the phase-transition properties of VO₂, the absorber demonstrated dynamic adjustability by modulating the absorption from 3% to 98.74%. The absorption mechanism was analyzed through the impedance matching theory and electromagnetic field distributions, confirming the role of magnetic resonance and interference. Furthermore, machine learning algorithms, specifically Linear Regression, Support Vector Regression, and Random Forest (RF), were applied to accelerate the design process and optimize the structural parameters. Among these, the RF model demonstrated superior prediction accuracy. The machine learning-assisted optimization successfully extended the effective absorption bandwidth to 9 THz, representing an improvement by 9.4% compared to the traditional optimization methods. These results validate the efficacy of combining electromagnetic simulation with data-driven techniques for advanced metamaterial design.

Keywords: metamaterial; broadband absorption; VO₂; machine learning



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1. Introduction

In the rapidly evolving landscape of modern technology, electromagnetic absorbers stand as critical components across diverse applications, from enhancing sensing systems [1,2] to optimizing emitters [3,4], and advancing thermophotovoltaic energy conversion [5,6]. In this technological area, metamaterials have emerged as a groundbreaking

innovation, drawing intense research interest and practical implementation due to their extraordinary capability for perfect electromagnetic absorption [7].

Unlike conventional materials, metamaterials yield their exceptional properties from precisely engineered subwavelength architectures that create resonant interactions with both electric and magnetic field components of incident electromagnetic waves [8]. These sophisticated structures consist of carefully designed “meta-atoms”—artificial electromagnetic building blocks that typically take the form of metallic split-ring resonators, intricately patterned wire meshes, complementary geometric arrangements, or other optimized configurations meticulously fabricated on dielectric substrates or embedded within them. The inherent versatility of metamaterial design enables unprecedented control over absorption frequency, bandwidth, and angular response, opening new possibilities for electromagnetic wave management across the entire spectrum from microwave to optical frequencies [9,10].

Practical applications of metamaterial absorbers not only demand high absorption rates but must also meet other criteria, such as broad bandwidth. Recent research on broadband absorbers has employed complex geometries [11], nano holes [12], or even graphene [13] to obtain these objectives. However, the use of composite materials is the most popular method to meet the requirements. As can be seen from the research by Chouhan et al., the proposed design offers an ultra-broadband bandwidth combined with the capability to modulate ultra-wideband THz amplitude caused by metal–insulator phase transitions in vanadium oxide thin films [14].

Furthermore, metamaterial structures can be modified through numerous design parameters to meet diverse requirements. The challenge lies in the complex relationship between design parameters and electromagnetic responses. Adjusting these parameters to achieve target responses essentially constitutes an optimization process that is time-consuming and labor-intensive. In recent years, machine learning (ML) has found applications across many fields thanks to its capability to learn from data, detect hidden features, and establish relationships between datasets [15].

This study numerically investigates a broadband metamaterial absorber (BMA) unit cell incorporating a VO₂ square patch to achieve dynamically tunable absorption characteristics across the THz regime. The investigated absorber not only offers the ability to adjust the absorption by changing the temperature-dependent conductivity of VO₂, but also features a simple configuration, thereby facilitating the fabrication process. Additionally, this work employs machine learning techniques to predict the absorption characteristics of the designed structure. Furthermore, it provides a comparison of different ML regressions and optimizes the geometric parameters.

2. Design and Simulation

The unit cell of the proposed absorber is shown in Figure 1, including three layers: VO₂–dielectric MF₂–Au. The top layer is made up of VO₂, which has a relative permittivity in the THz range, described by the Drude model [16]:

$$\varepsilon_{VO_2}(\omega) = \varepsilon_{\infty} - \frac{\omega_p^2(\sigma)}{(\omega^2 + j\gamma\omega)}, \quad (1)$$

where ω denotes the angular frequency of the incident electromagnetic wave, $\varepsilon_{\infty} = 12$ is the permittivity at very high frequencies, $\omega_p(\sigma)$ is the plasma frequency of VO₂, and $\gamma = 5.75 \times 10^{13}$ rad/s is the collision frequency constant. The relationship between $\omega_p(\sigma)$ and σ_{VO_2} can be expressed as

$$\omega_p^2(\sigma) = \frac{\sigma_{VO_2}}{\sigma_0} \omega_p^2(\sigma_0) \quad (2)$$

with $\sigma_0 = 3 \times 10^5$ S/m and $\omega_p(\sigma_0) = 1.4 \times 10^{15}$ rad/s. Upon exceeding a critical temperature of 68 °C, VO₂ undergoes a phase transition of insulator to a metallic state. When the metallic volume fraction $V_{(T)}$ is relatively large, the reduced spacing between particles makes inter-particle interactions significant. To be more specific, the dielectric constant of VO₂ can be expressed by the simple Bruggeman theory [17]:

$$\varepsilon_{VO_2(T)} = \frac{1}{4} \left(\varepsilon_D (2 - 3V_{(T)}) \right) + \varepsilon_M (3V_{(T)} - 1) + \sqrt{\varepsilon_D (2 - 3V_{(T)}) + \varepsilon_M (3V_{(T)} - 1)^2 + 8\varepsilon_D \varepsilon_M} \quad (3)$$

with $\varepsilon_D = 9$ of the VO₂ thin film dielectric function in the insulator state. ε_M is the permittivity of the metallic components in VO₂, expressed by the Drude model. Moreover, volume fraction $V_{(T)}$ of metal components can be explained by [18]

$$V_{(T)} = V \left(1 - \frac{1}{1 + \exp\left(\frac{T-T_0}{\Delta T}\right)} \right)_{max} \quad (4)$$

where $T_0 = 68$ °C is the phase transition temperature of VO₂ and $\Delta T = 3$ °C is the transition width [19]. From Equations (3) and (4), the conductivity of VO₂ can be expressed as $\sigma_{VO_2} = -i\varepsilon_0\omega(\varepsilon_{VO_2(T)} - 1)$. Furthermore, previous research demonstrated that the conductivity of VO₂ could be varied from 10 to 400,000 S/m through temperature adjustment [20]. The relationship between temperature and conductivity of VO₂ is demonstrated in Figure 2 through theoretical calculations. However, our study focuses on the change in VO₂ conductivity ranging from 200 S/m at 318 K to 200,000 S/m at 341 K.

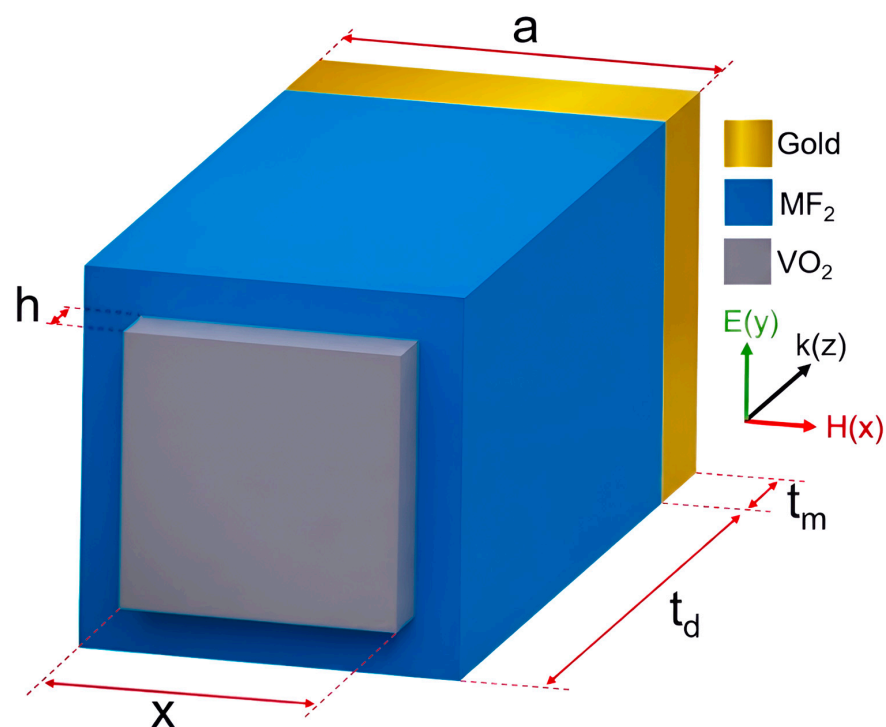


Figure 1. 3D schematic of the metamaterial structure with directions of the magnetic field, electric field, and wave vector.

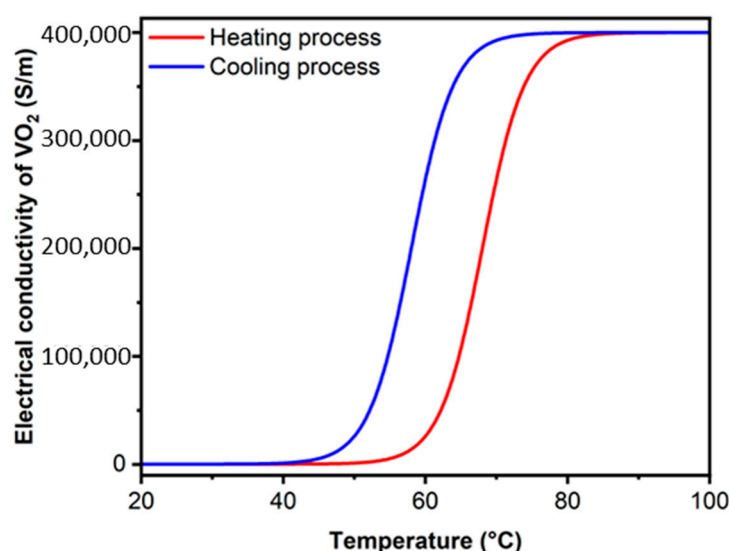


Figure 2. Temperature-dependent electrical conductivity of VO₂ film (heating process $T_0 = 68\text{ }^{\circ}\text{C}$, and cooling process $T_0 = 58\text{ }^{\circ}\text{C}$).

The middle dielectric is MF₂, a non-dispersive medium with a permittivity of 1.9 [21]. The metallic ground is made of gold, and its dielectric constant is characterized by the Drude model [22]:

$$\varepsilon_{Au}(\omega) = \varepsilon_0 - \frac{\omega_p^2}{\omega(\omega - i\tau)}, \quad (5)$$

where ε_0 represents the permittivity of free space, $\omega_p = 1.37 \times 10^{16}\text{ s}^{-1}$ is the plasma frequency of Au, and $\tau = 6.48 \times 10^{12}\text{ s}^{-1}$ is the damping rate. The simulation process was performed by using CST Studio Suite software 2023, with the structural parameters listed in Table 1.

Table 1. Parameters of the proposed unit cell.

Geometrical Parameters	a	x	t _m	t _d	h
Value (μm)	11	8	1	6	0.05

3. Results and Discussion

3.1. Electromagnetic Characteristics of VO₂-Integrated Broadband Absorption Materials

The simulated absorption, transmission, and reflection spectra of the BMA material at a conductivity of 200,000 S/m are illustrated in Figure 3a. The results exhibit two distinct absorption peaks at 6.1 and 11.91 THz, with absorption of 98.74% and 98.62%, respectively. Furthermore, the absorption bandwidth exceeding 90% is 8.23 THz, from 5.08 to 13.31 THz.

In addition, the relative bandwidth (RAB) is considered a quantity for comparing the broadband electromagnetic absorption performance of different BMA structures, regardless of their operating frequency ranges. It can be calculated by using the following formula:

$$RAB = \frac{2 \times (f_R - f_L)}{f_R + f_L}, \quad (6)$$

where f_R and f_L denote the upper and lower cutoff frequencies, respectively, at which the absorption remains above a specified threshold. For the investigated BMA structure, with the absorption threshold set at 89.5%, an RAB of 90% is obtained. As shown in Table 2, this represents a superior performance for a simple three-layer structure that is highly effective in broadband absorption.

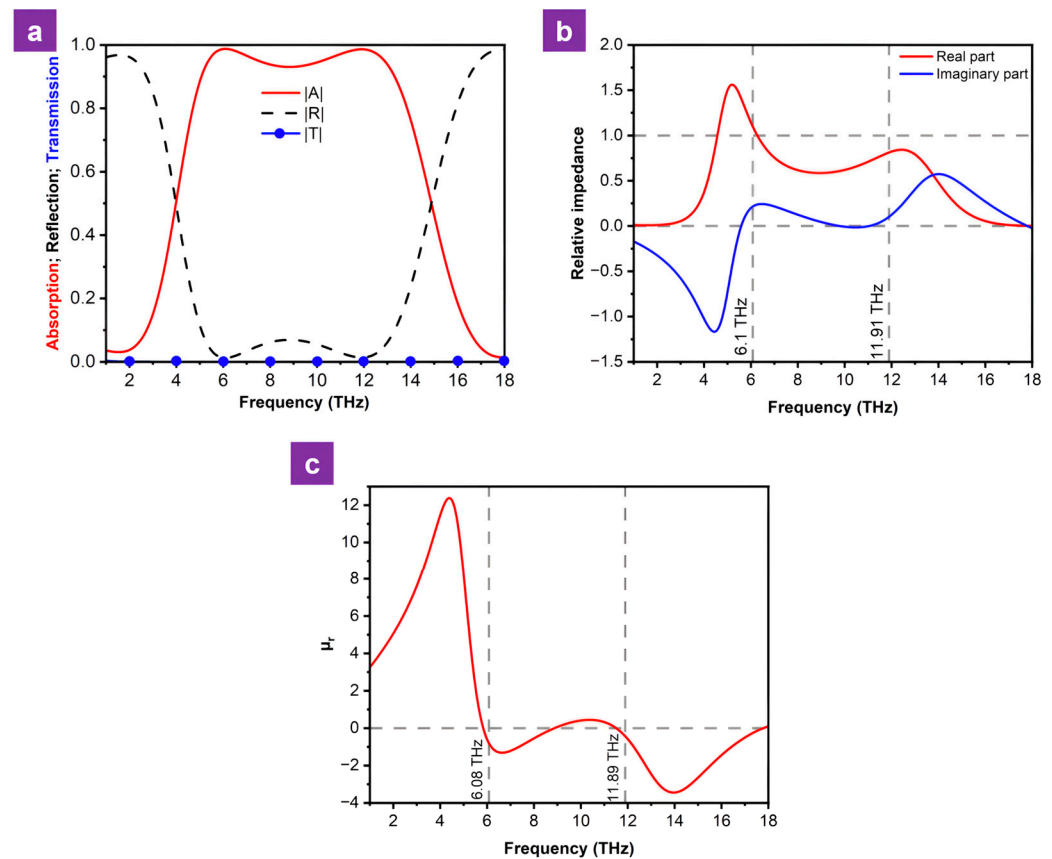


Figure 3. (a) Absorption, reflection, and transmission spectra, (b) relative impedance and (c) real part of the permeability at VO₂ conductivity of 200,000 S/m.

Table 2. Comparison of the proposed model with recent investigations.

Reference	Bandwidth	RAB	Absorption	Number of Layers	Structural Design and Composition
[23]	6.31 THz	77%	>90%	5	VO ₂ square patch and graphene loop
[24]	3.13 THz	85.4%	>90%	4	Square-shaped graphene and U-shaped VO ₂
[25]	0.75 THz	54.9%	>80%	3	VO ₂ micro-rod
[26]	6.62 THz	82.5%	>90%	3	VO ₂ hybrid structure
This work	8.23 THz	89.5%	>90%	3	VO ₂ square patch

The physical mechanism governing the electromagnetic absorption characteristics of the designed structure can be elucidated by employing the impedance matching theory. When electromagnetic waves propagate to the surface of a material, a portion of the energy is reflected into the free space, another fraction is transmitted through, and the remaining energy is absorbed by the material. The absorption $A(\omega)$ of the investigated model is calculated by using the following equation:

$$A(\omega) = 1 - R(\omega) - T(\omega), \quad (7)$$

where $T(\omega)$ and $R(\omega)$ represent the transmission and reflection, respectively. In this configuration, the continuous metal layer at the bottom serves to completely block the transmission of electromagnetic waves. Consequently, to maximize absorption, the reflection coefficient of the incident wave must be minimized. When the transmission is

neglected, the relationship between the absorption and the impedance of the material is expressed by the formula below:

$$A(\omega) = 1 - R(\omega) = 1 - \left| \frac{Z - Z_0}{Z + Z_0} \right|^2 = 1 - \left| \frac{Z(\omega) - 1}{Z(\omega) + 1} \right|^2. \quad (8)$$

Here, Z is the absolute impedance of the designed structure, and Z_0 is the impedance of the free space and can be calculated through permeability μ_0 and permittivity ϵ_0 : $Z_0 = \sqrt{\frac{\mu_0}{\epsilon_0}} = \sqrt{\frac{4\pi \times 10^{-7}}{8.854 \times 10^{-12}}} = 120\pi \Omega$. Additionally, the relative impedance $Z(\omega)$ can be expressed as [27]

$$Z(\omega) = \sqrt{\frac{\mu(\omega)}{\epsilon(\omega)}} = \sqrt{\frac{(1 + S_{11})^2 - S_{21}^2}{(1 - S_{11})^2 - S_{21}^2}}. \quad (9)$$

When the relative impedance $Z(\omega)$ approaches unity, the reflection nearly vanishes, thereby the optimal absorption of the proposed material is achieved. Based on the relative impedance calculated by Equation (9) and presented in Figure 3b, it can be observed that in a frequency range from 5.08 to 13.31 THz, the real part of the relative impedance varies between 1.5 and 0.5, while the imaginary part ranges from -0.8 to 0.3 . Specifically, at 6.1 THz, the real and imaginary parts of $Z(\omega)$ are 1.08 and 0.22, respectively, whereas at 11.91 THz these values are 0.81 and 0.1, respectively. These results demonstrate that, within the 5.08–13.31 THz band, the impedance of the material approximates that of the surrounding medium. Consequently, only a minimal fraction of the electromagnetic wave is reflected at the top interface, and transmission through the material is virtually nonexistent, as clearly evidenced by the transmission and reflection spectra in Figure 3a.

To further elucidate the resonance mechanism of the BMA, the electric field distributions on the surfaces of the Au and VO₂ layers when VO₂ is in the metallic phase are illustrated at the resonant frequencies of 6.1 and 11.91 THz in Figure 4. The simulation results indicate that, at 6.1 THz, the electric field vectors on the surfaces of the two layers are anti-parallel. Meanwhile, at 11.91 THz, the VO₂ layer exhibits three distinct regions where the electric field directions in adjacent zones are opposite. By correlating these electric field distributions with the calculated real part of the magnetic permeability presented in Figure 3c, it can be concluded that magnetic resonance is the primary origin of the two observed absorption peaks [28].

The incident angle of electromagnetic waves significantly influences the performance of metamaterial absorbers. Consequently, we simulated the effects of both TE and TM polarizations at varying incident angles on the absorption spectra. In general, the absorption peaks exceeding 90% exhibit significant angular stability, remaining largely insensitive to the incident angle for values up to 60°, while the broadband absorption performance remains stable for incidence angles up to 30° under TE polarization and extends to 40° for the TM mode. As can be seen in Figure 5, when the incidence angle increases further to 80° for both polarization modes, the absorption peaks in the TM mode are significantly better preserved than those in the TE mode. This superior stability is attributed to the inherent magnetic resonance nature of the peaks, which remains more robust under TM excitation.

To investigate the influence of the phase-change material VO₂ on the electromagnetic properties of the BMA structure, the absorption spectrum was simulated across different VO₂ conductivities. As illustrated in Figure 6a, increasing the VO₂ conductivity from 200 to 200,000 S/m results in a variation in absorption changing from 3% to 98.74%, with the center frequency remaining nearly unchanged. Moreover, Figure 6b demonstrates that the absorption characteristics of the metamaterial can be actively controlled through thermal regulation of the VO₂ layer. By modulating the temperature, the device can be effectively switched from a transparent state to a near-perfect absorbing one, demonstrating high

sensitivity to the VO₂ phase transition. The observed phenomenon is due to the dependence of the dielectric constant of VO₂ on its electrical conductivity. Based on Equations (1) and (2), the imaginary part of the dielectric constant VO₂ for different conductivities is shown in Figure 6c. It can be seen that, as the conductivity of VO₂ increases, the imaginary part ϵ'' of the dielectric constant also increases sharply in its magnitude, and the energy loss density is expressed by the following equation [29]:

$$P_{loss} = \frac{1}{2} \omega \epsilon'' |E(\omega)|^2 \quad (10)$$

with ω and $E(\omega)$ are the angular frequency and electric field intensity of the incident wave, respectively. According to the expression above, the energy loss density is directly proportional to the imaginary part of the dielectric constant, which explains why, when VO₂ gradually transitions to the metallic phase; thereby, the overall absorption of the designed metamaterial is enhanced.

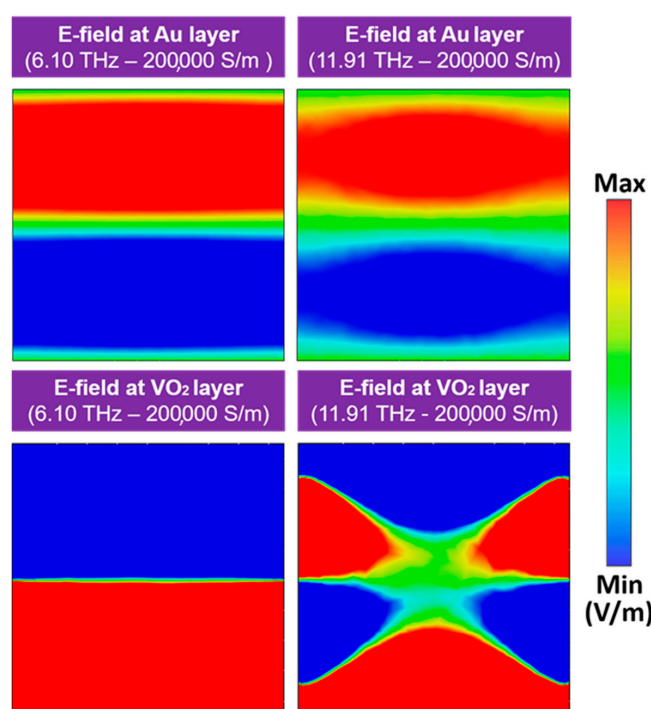


Figure 4. Electric field distribution on the Au layer and the VO₂ one at a conductivity of 200,000 S/m for two resonance frequencies: 6.10 and 11.91 THz.

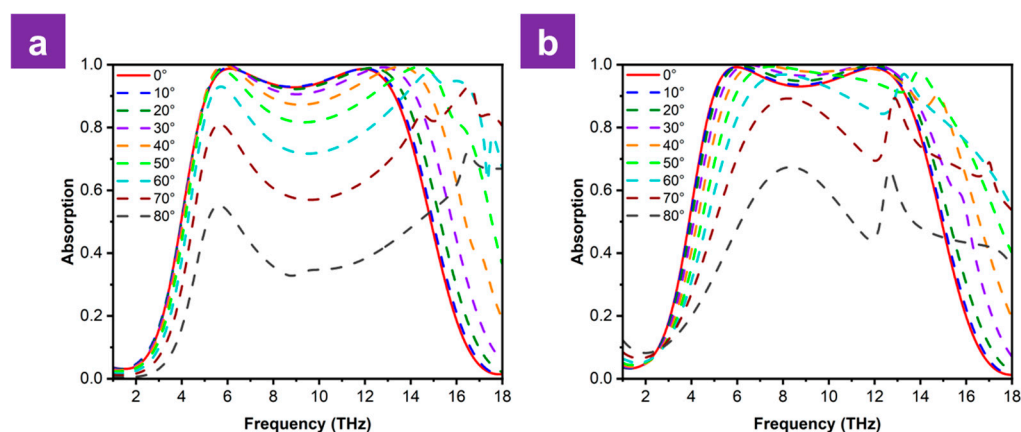


Figure 5. Performance of the absorber under (a) TE and (b) TM polarization.

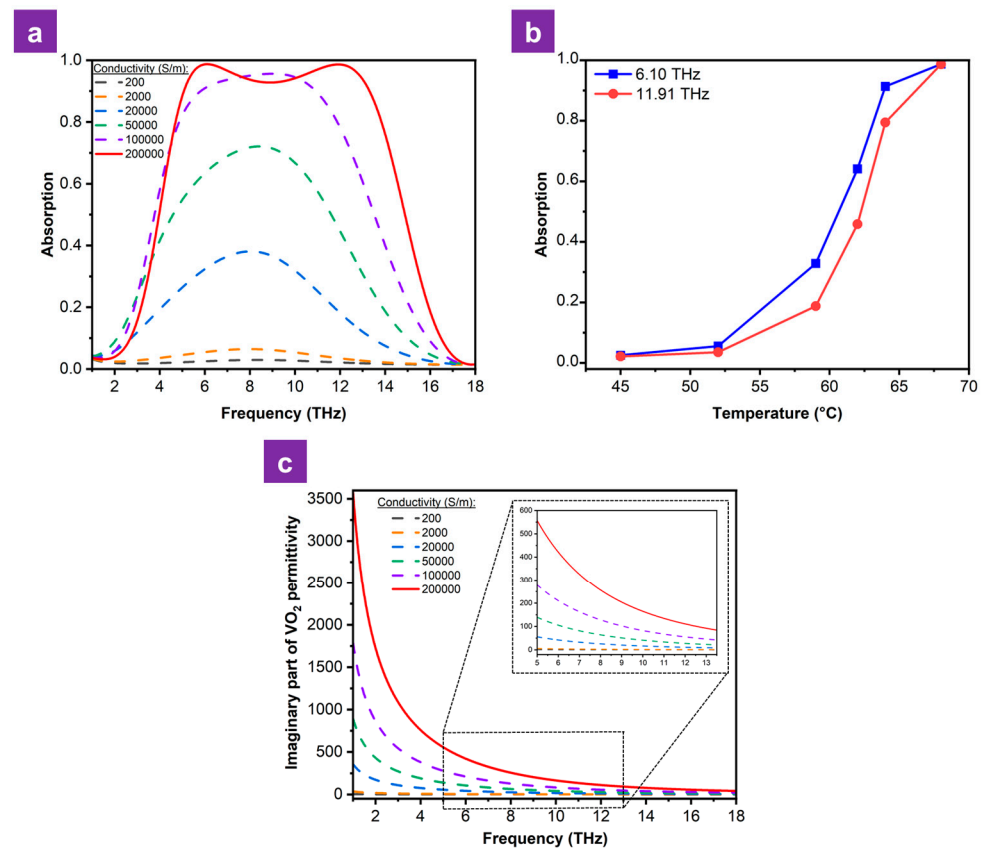


Figure 6. (a) Absorption spectra and (c) imaginary parts of the dielectric constant of VO₂ at different conductivity levels. (b) Temperature-dependent absorption for the resonance peaks of 6.10 and 11.91 THz.

The electric field energy density for different conductivities of VO₂ at 6.1 and 11.91 THz was simulated to understand the mechanism of switching between reflection and absorption of the investigated structure, which is shown in Figure 7. When VO₂ is in the insulator phase, specifically at conductivity values of 200 S/m, 2000 S/m, and 20,000 S/m, the electric field energy density remains low and distributes almost uniformly. This indicates that no resonance occurs at these conductivities, where the investigated structure primarily acts as a reflector. As can be seen, when VO₂ transitions to the metallic phase, the electric field energy is strongly concentrated at the edges of the square, especially the top and bottom edges of the VO₂ layer. This simulation result demonstrates that, when the conductivity of VO₂ is 200,000 S/m, there are more free electrons in the VO₂ layer, and these electrons oscillate under the excitation of the incident electromagnetic wave, leading to the generation of surface currents. This phenomenon forms resonance peaks at two frequencies, 6.10 and 11.91 THz, which helps to increase the performance of absorbers.

The performance of an absorber is highly sensitive to its geometric parameters; therefore, parameter optimization is crucial in obtaining the optimal performance. Figure 6 illustrates the influence of structural parameters on the absorption spectrum at a conductivity of 200,000 S/m. Figure 8a reveals that increasing the width x from 6 to 8 μm broadens the absorption bandwidth and increases the maximum absorption toward unity. As the width x continues to increase to 10 μm , the first resonance peak gradually shifts towards a lower frequency, whereas the second one experiences a blue shift. Although these shifts result in a broadening of the absorption spectrum, they lead to a degradation in absorption within the central frequency region, causing the structure to lose its broadband absorption characteristic. Thus, $x = 8 \mu\text{m}$ is chosen as the optimum value.

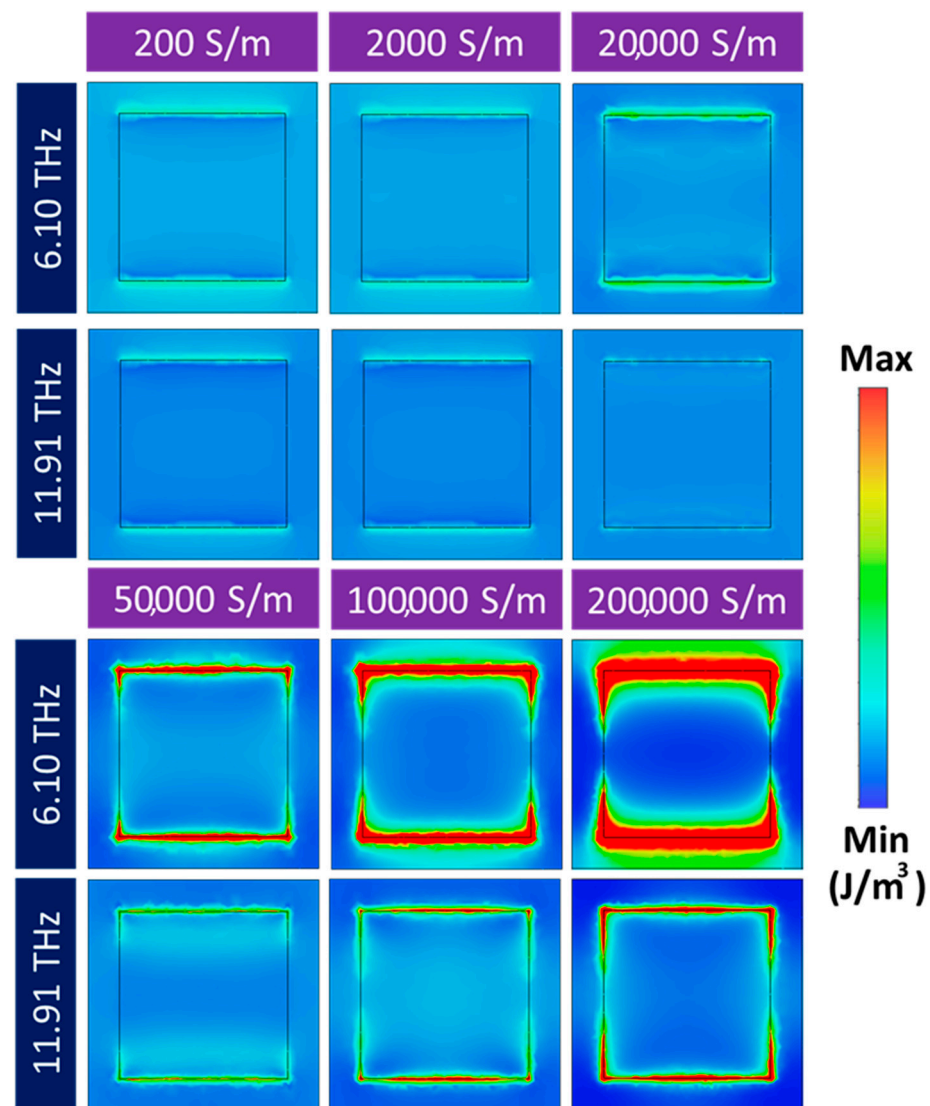


Figure 7. Simulated electric field energy density at frequencies of 6.10 and 11.91 THz for different electrical conductivities of VO₂.

Subsequently, the simulation results for different thicknesses of the VO₂ layer are shown in Figure 8b. As the dielectric layer thickness h changes from 0.015 μm to 0.05 μm , both the absorption and the absorption spectrum are gradually enhanced. While the resonance peaks remain stable as the thickness increases up to 0.1 μm , the absorption itself exhibits a decline. This is caused by the degradation of impedance matching between the investigated structure and free space. Therefore, 0.05 μm is identified as the optimum thickness to guarantee the near-perfect impedance matching.

The absorption spectrum of the absorber depends on the dielectric layer thickness, as shown in Figure 8c. The simulation results show that, while the position of the first resonance peak remains almost unchanged, the second one exhibits red shifts as the dielectric layer thickness increases. For an optimized dielectric thickness of 6 μm , the center frequency of the absorption spectrum is approximately 9.19 THz, corresponding to a vacuum wavelength of 32.64 μm . Because the refractive index of the dielectric layer is $n = \sqrt{\epsilon} = \sqrt{1.9} \approx 1.37$, the wavelength in the dielectric layer decreases to approximately 23.82 μm . This absorption mechanism can be explained by the interference cancellation principle. When the dielectric layer thickness is approximately one-quarter of the wavelength in the dielectric layer, it satisfies the condition of canceling interference between the reflected

and incident waves, allowing the proposed structure to obtain a broadband absorption of over 90%. As a result, the absorber shows strong absorption at this specific thickness.

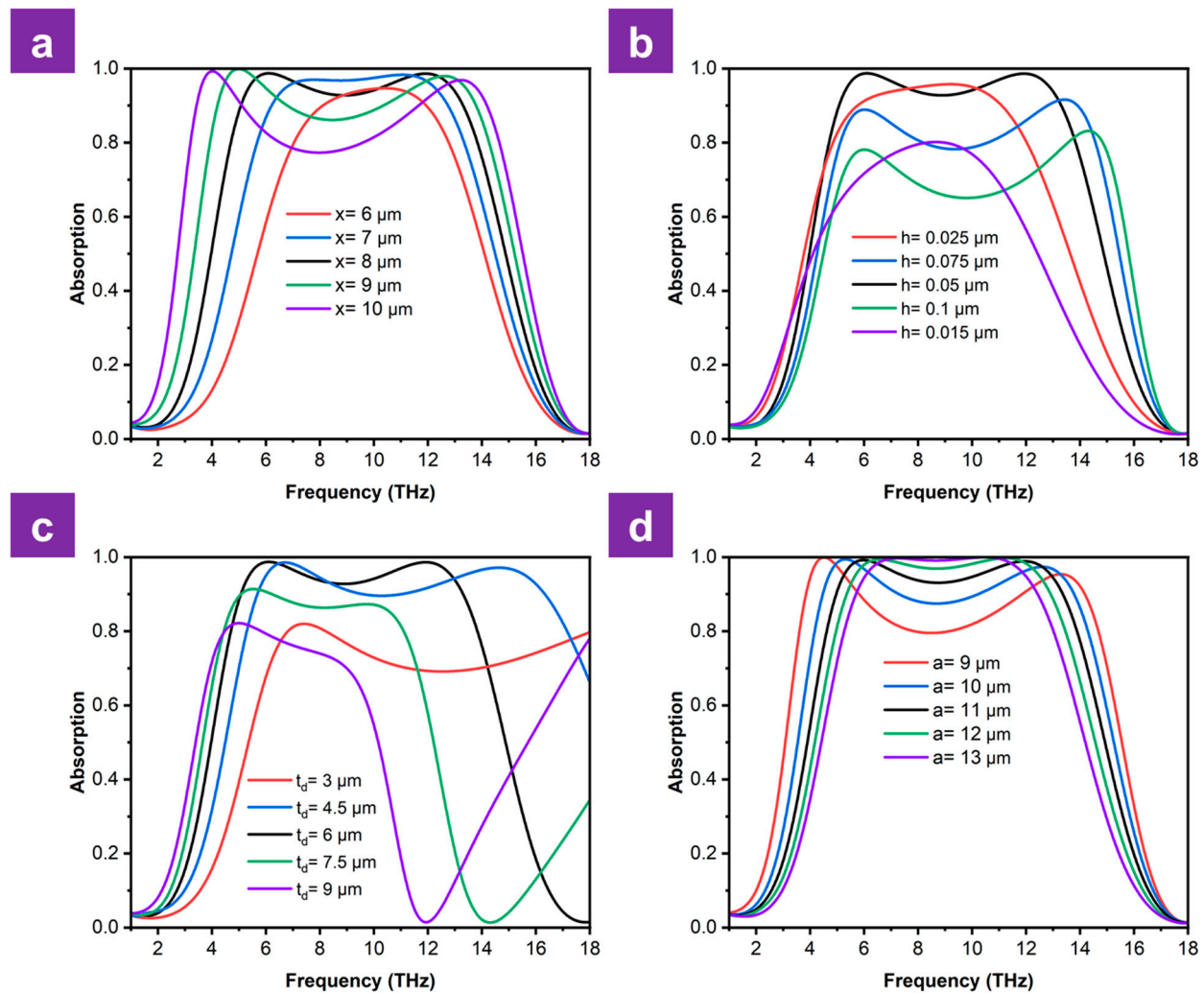


Figure 8. Variation in absorption spectra according to (a) VO₂ layer size, (b) VO₂ layer thickness, (c) dielectric layer thickness and (d) unit cell period.

As the unit cell period a of the metamaterial increases from 9 to 13 μm , the absorption spectrum demonstrates a clear trade-off between bandwidth and absorption stability above the 90% threshold, shown in Figure 8d. At the smallest period ($a = 9 \mu\text{m}$), the structure fails to maintain a continuous 90% absorption, since a significant dip occurs in the center of the band where absorption falls to approximately 80%. A gradual increase in the unit cell period causes the first resonance peak to exhibit a blueshift, whereas the other peak exhibits a redshift. This phenomenon initially facilitates a broadband absorption capability within the structure. However, as the period is further increased up to 13 μm , this trend persists, ultimately leading to a contraction of the bandwidth where absorption exceeds 90%. As evidenced in Figure 8d, a unit cell period of 11 μm yields the optimal bandwidth for high-efficiency absorption.

3.2. Machine Learning Prediction Results

Figure 9 illustrates the process of using an ML model trained by a dataset consisting of 2010 data points. This process began with simulating and exporting data from CST software, followed by labeling and scaling the data. After preprocessing, the dataset was split into a test sample (20%) and a training one (80%). Finally, the results predicted by the

ML model are compared with the simulation results by CST. To clarify, the 2010 data points were generated by using a parametric sweep sampling strategy via CST simulations. The parameter space was covered uniformly to avoid any sample imbalance. Specifically, the parameter x was sampled to be 1 to 11 μm with a step size of 0.05 μm (201 points), and the parameter h was sampled from 0.01 to 0.1 μm with a step size of 0.01 μm (10 points). Three regression models were used: Linear Regression (LR), Support Vector Regression (SVR), and Random Forest (RF). LR was employed as a baseline to evaluate the linearity of the design space. For SVR, a radial basis function kernel and an ε -insensitive loss function were utilized to capture non-linear characteristics, while the RF model was trained by minimizing the mean squared error loss function. To ensure optimal predictive accuracy and prevent overfitting, a grid search strategy was performed for hyperparameter optimization. Model performance was rigorously evaluated by using the coefficient of determination, mean absolute error, and mean squared error. The targets are the absorption bandwidth with absorption above 50% and 90%.

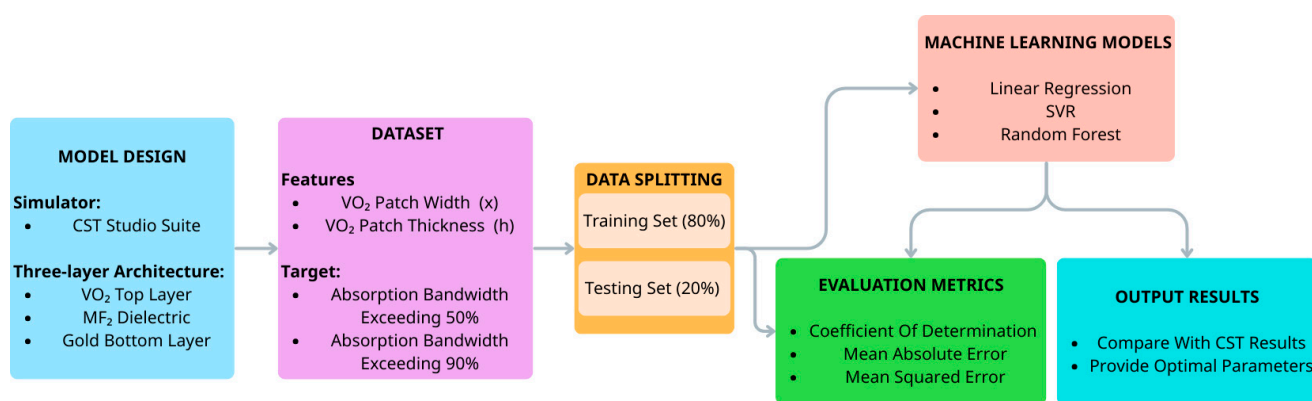


Figure 9. Flow chart showing the workflow of the proposed study.

Based on evaluation metrics including R^2 , MAE and MSE shown in Table 3, it is possible to provide a comprehensive assessment of the performance of three ML models. Among the three algorithms, the Linear Regression model exhibits the worst performance. Specifically, R^2 values on the test set reach only approximately 0.855 and 0.280 for predicting the absorption bandwidth exceeding 50% and 90%, respectively. Moreover, the error parameters for both output results are also relatively high, with MAE values of nearly 1.48 and 1.46, and MSE values of around 3.79 and 4.26 on the test set. In contrast, the SVR model presents significantly better performance than the LR model, with the R^2 values on the test set improving strongly, reaching 0.987 and 0.981 for the two target variables. Furthermore, both MAE and MSE values on the test set decrease substantially, demonstrating a superior capability in modeling non-linear features.

Table 3. Evaluation metrics for ML models. MAE is the mean absolute error, and MSE is the mean squared error.

Output Results	Linear Regression	SVR	Random Forest
Absorption Bandwidth Exceeding 50%	R^2 : 0.855 MAE: 1.48 MSE: 3.79	R^2 : 0.987 MAE: 0.26 MSE: 0.34	R^2 : 0.9991 MAE: 0.057 MSE: 0.024
Absorption Bandwidth Exceeding 90%	R^2 : 0.280 MAE: 1.46 MSE: 4.26	R^2 : 0.981 MAE: 0.17 MSE: 0.11	R^2 : 0.9982 MAE: 0.040 MSE: 0.011

However, RF outperformed the others. R^2 values on the testing dataset approach unity for both output results, and the error metrics are all less than 0.06, indicating high predictive accuracy and robust generalization capability. Notably, the minimal divergence between the evaluation parameters on the training and test sets, as presented in Table 4, illustrates that the model effectively mitigates overfitting. This advantage is attributed to the nature of the RF algorithm, which aggregates predictions from multiple decision trees, thereby reducing variance and enhancing model stability.

Table 4. Comparison of R^2 , MAE and MSE values on training and validating dataset for RF model.

Output Results	R^2 Values on Training/Validating Dataset	MAE Values on Training/Validating Dataset	MSE Values on Training/Validating Dataset
Absorption Bandwidth Exceeding 50%	0.9998/0.9991	0.023/0.057	0.004/0.024
Absorption Bandwidth Exceeding 90%	0.9997/0.9982	0.014/0.04	0.002/0.011

To evaluate the accuracy of the proposed ML approach, we analyzed the relationship between the predicted outcomes and the simulated results in the testing dataset. Figure 10 illustrates the scatter plots for the absorption bandwidths at the 50% and 90% thresholds. The tight alignment of the test samples along the diagonal line confirms that the RF effectively captures the non-linear relationship between the geometric parameters and absorption performance. To further clarify the actual accuracy of the model by using the RF algorithm, the prediction results are compared with some simulation results (not included in the test set) by employing the CST software, and are shown in Table 5. Based on the comparison table of the simulation and prediction results, the RF model shows fairly high accuracy in most cases, with relatively small errors. In particular, the model predicts with absolute accuracy in cases where the absorption bandwidth is 0 THz.

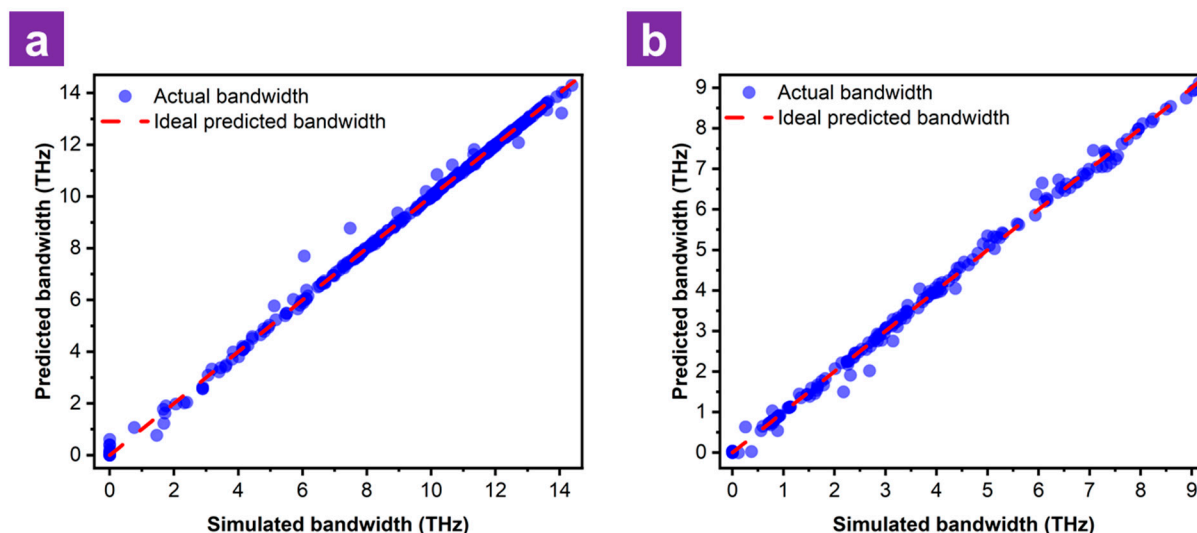
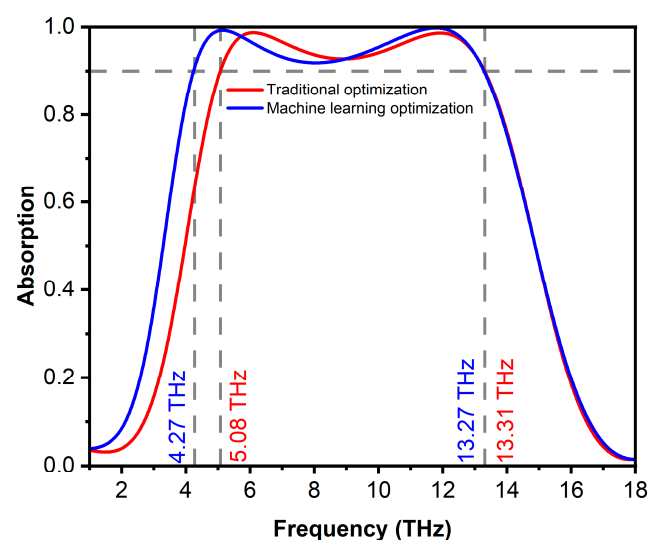


Figure 10. Scatter plots of RF show the relationship between the predicted and simulated values (blue dots) of (a) absorption bandwidth above 50% and (b) absorption bandwidth above 90% in the testing dataset. The red dashed line represents the ideal fit of the absorption bandwidth.

Table 5. Comparison of simulated and predicted values by using CST software and RF model, respectively.

Input Parameters (μm)	Predicted/Simulated Absorption Bandwidth Above 50% (THz)	Error	Predicted/Simulated Absorption Bandwidth Above 90% (THz)	Error
$x = 7.37$ $h = 0.01$	4.38/4.65	5.8%	0/0	N/A
$x = 8.69$ $h = 0.019$	10.15/9.89	2.6%	2.17/1.94	11.8%
$x = 7.87$ $h = 0.04$	10.68/10.5	1.7%	7.79/7.56	3.04%
$x = 7.8$ $h = 0.12$	11.33/11.08	2.3%	0/0	N/A
$x = 9.46$ $h = 0.045$	12.43/12.3	1.1%	5.28/5.77	8.4%

After successfully training the RF model, a grid of input values is generated to find the optimal parameters. To be more specific, the predicted results are analyzed to identify the pair of structure parameters reaching the maximal absorption bandwidth above 90%. The obtained parameters are $x = 8.96 \mu\text{m}$ and $h = 0.04 \mu\text{m}$, corresponding to a predicted bandwidth of 9.19 THz. As shown in Figure 11, the actual simulation result for these parameters yielded a bandwidth of 9 THz, representing a 9.4% improvement compared to the optimal result obtained by the traditional method. Moreover, the ML approach reduces the total computational time by several orders of magnitude while ensuring a more comprehensive exploration of the design space. Generating 2010 samples required approximately 4020 min of simulation time. Once the model is successfully trained, it can instantaneously predict the bandwidth for both 50% and 90% absorption for any new set of structural parameters and provide the optimal parameters.

**Figure 11.** Simulated absorption spectra of the optimal structure by using the traditional method and ML techniques.

4. Conclusions

This study simulates and investigates a broadband metamaterial absorber integrated with vanadium dioxide operating in the THz regime. The simulation results demonstrate

a wide absorption bandwidth of 8.23 THz (spanning from 5.08 to 13.31 THz), with the capability to modulate absorption from 3% to 98.74% by varying the conductivity of the VO₂ layer. Specifically, at a conductivity of 200,000 S/m, two magnetic resonance peaks emerge at 6.1 and 11.91 THz, satisfying the impedance matching condition with the free space and enabling a broadband absorption within the operating frequency range. In addition to structural design, this paper confirmed the efficacy of applying ML to accelerate the design process. Among the three algorithms investigated, RF demonstrated superior performance by accurately capturing complex non-linear relationships that Linear Regression failed to address. The machine learning algorithm not only provided predictions closely aligned with the simulation results but also optimized the structural parameters more effectively than manual tuning methods, resulting in a 9.4% improvement in the absorption bandwidth.

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