Invited Paper

Design and optimization of terahertz filter devices based on deep learning

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Abstract: In order to meet the demand for efficient design of terahertz functional devices, this paper starts from the target function of the device and quickly and accurately designs the desired filter structure. The design of conventional metasurface electromagnetic filters is relatively cumbersome, and it is difficult for manpower alone to complete a large amount of data analysis. The whole process wastes time and consumes computing resources. How to quickly and accurately design and optimize metasurface electromagnetic filters has become a major problem in the current field of metasurface research. Although machine learning is currently widely studied in the field of metasurfaces, there are few studies on metasurface electromagnetic filters using machine learning. Since electromagnetic filters have strong practical value and in order to avoid the shortcomings of conventional design methods, this paper uses deep learning to study metasurface electromagnetic filters. In addition, a forward spectrum prediction network and a reverse structure prediction network are designed using convolutional neural networks. The prediction results show that deep learning can well learn the physical relationship between the spectrum and structure of terahertz filters, which will greatly reduce the design time of researchers.

Keywords: Reverse design, Terahertz metasurface, Deep learning, Neural network

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1. Introduction

Terahertz (THz) waves are usually defined as electromagnetic waves with a frequency range between 0.1 and 10 *THz*. They have many special properties, such as strong penetration, low energy, frequency selectivity, etc. Previously, due to the lack of effectiveness, Terahertz wave generation and detection methods have not been fully developed. In recent years, with the development of terahertz science and technology, related terahertz devices, such as isolators [1], filters [2], liquid crystal substrate metasurfaces [3], on-chip devices [4], etc., have mushroomed. At present, terahertz technology has been widely used in satellite communications [5], biomedicine [6], materials science [7], physical chemistry [8] and other fields. The design of traditional terahertz functional devices usually relies on forward design methods, which have very high requirements on the experience of researchers. Designers need to master in-depth knowledge of optical theory and gradually approach the expected design goals by repeatedly debugging the characteristic parameters of the unit structure under the structural template of the existing device. Traditional design methods have significant limitations, consume a lot of time and energy, are limited by the setting of parameter space, and often can only obtain suboptimal design results. Although the forward design method has been widely used in the field of terahertz functional device design, its limitations have prompted researchers to explore more efficient and intelligent design methods to improve the accuracy and efficiency of the design.

In recent years, reverse design methods have shown great potential in the design of metasurface devices. With the advantages of intelligent design and full-space design freedom, reverse design transcends traditional theory and experience, especially in the design of photonic devices with ultra-small size, ultra-high performance and innovative functions. The reverse design method uses artificial intelligence algorithms to optimize the structure of optical devices. Unlike traditional forward design, reverse design starts from the target function and looks for a structure that meets the requirements. In the reverse design of mainstream optical devices [9], the application of artificial intelligence algorithms can be roughly divided into two design modes: heuristic algorithms based on groups and machine learning algorithms based on data sets. For example, genetic algorithms were used to iteratively design metamaterial absorbers [10-12] and multi-channel focusing wavelength demultiplexers designed based on target priority algorithms [13]. Liu et al. [14] proposed a series network structure and designed a multi-layer film structure composed of an alternating combination of SiO2 and Si3N4 to prove the feasibility of the series neural network. Peurifoy et al. [15] used a deep neural network (DNN) to predict the light scattering of multilayer core-shell nanoparticles composed of silica and titanium dioxide. Ma [16] et al. used the metamaterial on-demand design method of bidirectional neural network to achieve bidirectional prediction between key parameters and electromagnetic response of open ring metamaterials. The trained network successfully predicted the structural parameters of the desired spectrum, and the predicted spectrum. It has good consistency with the expected spectrum, indicating that the neural network can solve the reverse design problem more accurately. Group-based heuristic algorithms, such as Direct Binary Search Algorithm (DBS) [17], Genetic Algorithm (GA) [18] and Particle Swarm Optimization (PSO) [19], etc. etc., need to be linked with simulation software to perform complex simulation calculations. In contrast, the reverse design of optical devices based on deep learning methods does not require complex simulation modeling work, nor does it need to scan and calculate various parameters. A neural network needs to be built to learn the relationship between different metasurface structural parameters and their corresponding electromagnetic response characteristics, so that the electromagnetic characteristics of any metasurface can be simulated. Although the neural network can quickly design the target structure after training, the construction of huge data sets takes a lot of time. In the process of iterative optimization using heuristic algorithms, the heuristic algorithm continuously explores and converges in the search space, which will generate a large amount of local optimal solution or suboptimal solution data. This article collects these data sets and uses them in deep learning. During training, the required data set is quickly built and expanded in the process. By continuously accumulating local optimal solutions and optimal solutions, the diversity and coverage of the data set can be effectively improved.

Using heuristic algorithms as a way to obtain data sets, this paper independently builds a convolutional neural network and proposes a network scheme for terahertz metasurface design. This article takes the terahertz filter, an important component of the spectrum analysis system/imaging, as a research case to carry out the design and optimization of terahertz filter devices based on deep learning. The research results show that the convolutional neural network black box model built in this article can be based on the input of the spectral response. Data generation is required for functional terahertz filters.

2. Deep learning design methods

2.1 Building a Dataset

The data set is one of the core elements of training deep neural networks. The size and quality of the data set will directly affect the final training effect of the network. This paper explores the research on the terahertz filter metasurface. Therefore, the data set of this paper consists of two parts: one is the structural parameters of the terahertz filter metasurface, and the other is the spectral response curve of the metasurface corresponding to the structural parameters in the terahertz band.

In order to improve the efficiency of data acquisition and reduce the burden on researchers, the finite difference time domain method FDTD [20] and MATLAB co-simulation method are used to replace manual simulation. In the FDTD software, since it has a MATLAB program interface, the constructed model can be saved as a file and run in MATLAB. MATLAB will call the FDTD library function for calculation during the execution of the heuristic algorithm, and the data set can be collected during this process.

In order to facilitate the data input of the network, the metal layer of the frequency selective surface (FSS) is first divided into 20 × 20 blocks. Then, the structural parameters of the FSS unit are set: the unit period is 400 μm, the thickness is 10 μm, the material is selected as aluminum, and 10 μm thick polyimide is selected as the substrate. Due to space limitations, the specific model construction and heuristic algorithm are not elaborated in detail. The specific model diagram and heuristic algorithm can refer to the research results of reference [21]. Finally, in order to facilitate the access to the convolutional layer and the predicted symmetry, the 1/4 structure of the metal layer is selected as the input of the network. Finally, 16985 sets of data were collected. After completing the collection of the data set, the neural network training began.

2.2 Forward prediction network training

This section introduces the forward prediction neural network based on the terahertz filter metasurface. The computer processor used is the 12th Gen Intel(R) Core(TM) i5-12400f@2.50 *GHZ*, the GPU model is NVIDIA Ge Force RTX 3050, the deep learning framework is the PyTorch framework that supports GPU acceleration, and the integrated development environment is Jupyter Notebook. The input of the forward model is the 0, 1 structure matrix of the terahertz filter, and the output is the spectrum response parameter. The complete forward prediction neural network is shown in Figure 1, which consists of an input layer, a convolutional layer [22], a fully connected layer, and an output layer.

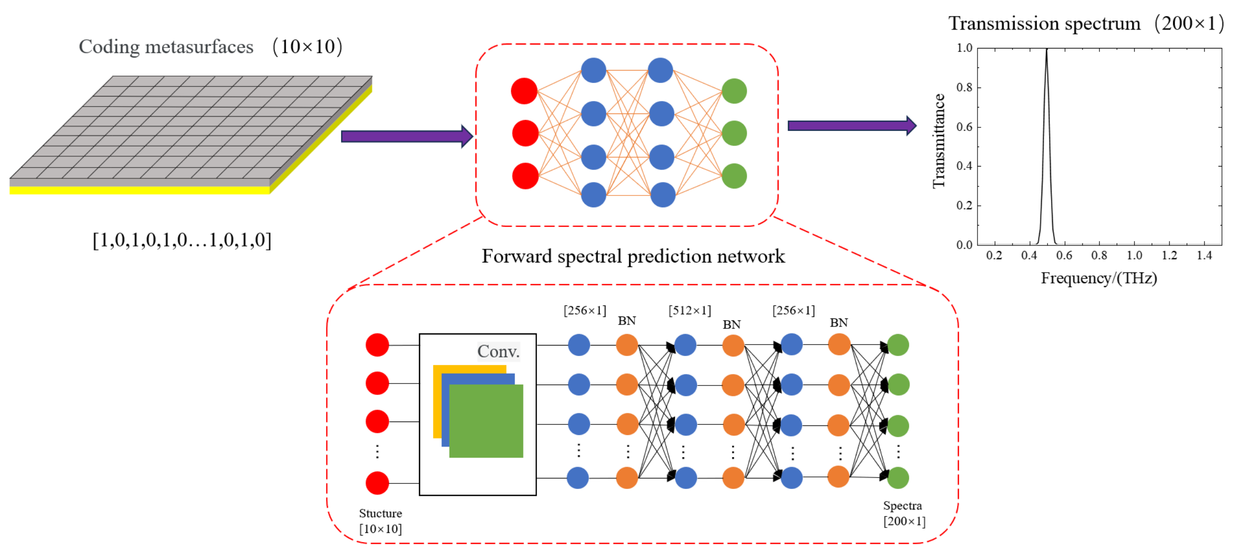

Fig.1 Forward prediction network structure schematic diagram

Throughout the network construction process, a matrix of size 10×10 is input and fed into the first convolutional layer. In order to extract the structural features of the hypersurface, a 3×3 convolution kernel is selected in the convolution layer. Next, a pooling layer [23] is used, with a size of 2×2. The main role of the pooling layer is to reduce the size of the feature map through downsampling while retaining important feature information as much as possible. After three convolution and pooling operations, the 10×10 matrix is converted into a 256×1 format, thereby achieving effective feature extraction and compression of the original data. This operation not only retains key structural information, but also significantly reduces the amount of data, making subsequent calculations more efficient.

After the aforementioned operations are completed, the obtained one-dimensional vector data is input into the subsequent fully connected layer. By adjusting and optimizing the hyperparameters, a deep neural network composed of three fully connected layers was constructed, in which the number of neurons in each layer was 256, 512 and 256 in sequence. After each fully connected layer, batch normalization (BN) [24] is introduced. The main function of the BN layer is to standardize the input data and adjust the data distribution through translation and scaling operations, which helps to alleviate the over-fitting problem and improve the training efficiency and stability of the network. Through this series of structural design and parameter adjustment, effective learning and expression of input data are achieved, further enhancing the model's prediction ability and training effect. The last layer is the output layer, which consists of 200 neurons and represents 200 spectral points of the output spectral response parameters. In the built forward prediction neural network, the rectified linear unit function [25] (ReLU) is used as the activation function, and its mathematical expression is:

$$f(x) = \max\{0, x\} \tag{1}$$

In the formula, when the input is less than 0, the function output is 0; when the input is greater than or equals to 0, the function output is the input itself. The advantage of the ReLU function is that its gradient is discrete, which is 0 or 1, and there is no gradient vanishing problem, which makes the neural network converge faster.

During the network training stage, the mean square error loss function [26] (MSE) is used for training and parameter learning. It represents the average of the square of the difference between the predicted value and the actual value. It is sensitive to errors and helps to find the model with the minimum error. Generally speaking, the smaller the MSE, the better the prediction ability of the model. The calculation formula of MSE is as follows:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(T_{prediction} - T_{simulation})^2 \tag{2}$$

Where $T_{prediction}$ is the predicted spectrum and $T_{simulation}$ is the actual FDTD simulated spectrum.

In the experiment of this paper, the collected 16985 sets of data are randomly shuffled, and the random seed is set to 0. The data set is divided into training set, test set and validation set in proportion, with the proportions of 80%, 10% and 10% respectively. In the setting of network parameters, the batch size is set to 128, that is, each batch contains 128 data samples, and the learning rate is set to 0.00001. According to the results of Figure 2(a), when the convolutional layer and the fully connected layer are both 3 layers, the network loss reaches the lowest. As shown in Figure 2(b), after 600 epochs of training, the loss value of the final model on the training set is 0.0005, and the loss value on the validation set is 0.0022. This result shows that under this configuration, the network achieves good convergence effect and high generalization ability. Through this series of experimental design and parameter adjustment, the effectiveness and accuracy of the network in processing such data are verified.

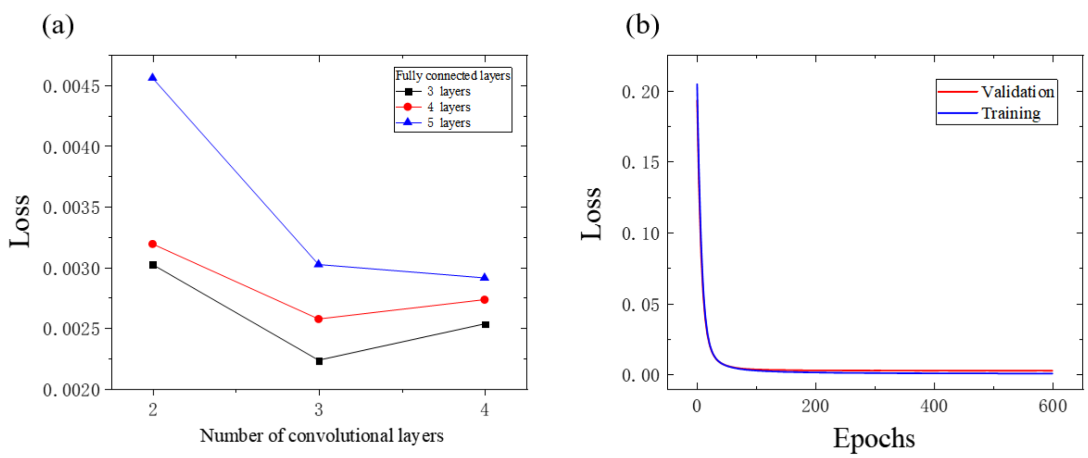

Fig. 2 (a) Loss comparison of different network structures; (b) Forward network loss function change curve

2.3 Reverse prediction network training

After the training of the forward prediction network is completed, the reverse network can be connected in series to the front of the forward network to form a cascade network for training. It should be noted that the forward network is mainly used for simulation during training, so its parameters should remain fixed. To achieve this goal, the weight parameters of the forward network are frozen and do not participate in the training process. The parameters of the reverse network will be continuously adjusted during the training process. In other words, the parameters of the forward network are set to a non-trainable state. The input of the reverse network is the target spectrum response data, and the output is the 0, 1 structure matrix of the terahertz filter metasurface designed by the neural network. The data set used by the reverse design neural network is the same as that of the forward network. The reverse design network structure is shown in Figure 3, which consists of a convolutional layer, a leaky ReLU[27-32], a pooling layer, and a fully connected layer.

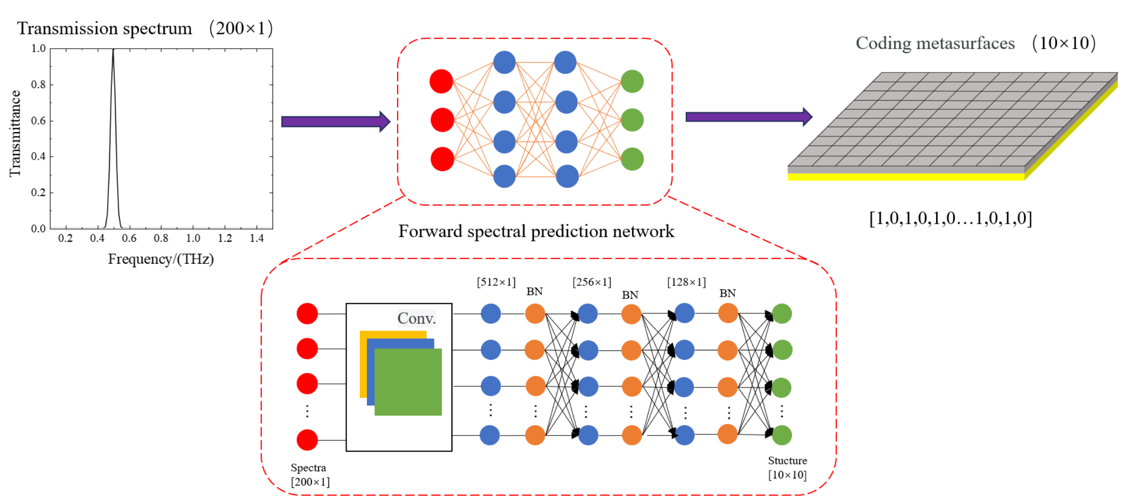

Fig. 3 Reverse prediction network structure diagram

In this network, Adam is selected as the optimizer. The key to the Adam optimizer is to simultaneously calculate the exponential moving average of the first-order moment of the gradient (i.e., the exponential weighted average of the gradient, usually called momentum) and the second-order moment (i.e., the exponential weighted average of the square of the gradient), and perform bias correction on them to ensure that the gradient estimate will not be biased towards 0 in the early stages of training, so that the learning rate is automatically adjusted, thereby improving the learning effect of the network. In addition, the Sigmoid function is used in the output layer of the network. The Sigmoid function can transform the input into data between 0 and 1. Its mathematical expression is as follows:

$$f(x) = \frac{1}{1+e^{-x}} \tag{3}$$

It is usually used in binary classification problems. The closer the output value is to 1, the greater the probability that the sample belongs to a certain category. The closer the output value is to 0, the greater the probability that the sample belongs to another category.

In the process of network construction, the input is 200×1 spectrum response data. After a layer of convolution and pooling calculation, it is flattened into a one-dimensional vector and connected to the fully connected layer. This paper constructs a fully connected layer with a depth of 3 layers, and the corresponding number of neurons is 512, 256, and 128. BN layers are added after each fully connected layer. The last layer is the output layer, which consists of 100 neurons, indicating that the dimension of the network designed is 10×10. Then set the random seed seed to 0. Among the 16985 sets of data sets used by the reverse prediction network, 80% are used as training sets, 10% as test sets, and 10% as validation sets. In the parameter setting of the network, Epoch is set to 1000, batch size is set to 64, learning rate is 0.0001, and MSE is still selected as the loss function. In the process of network training, overfitting occurs. Therefore, in order to reduce the overfitting phenomenon, a Dropout layer is added to the fully connected layer and set to 0.5. It is a regularization technique used to prevent neural network overfitting. It means that each time during the training process, 50% of the neurons (including their connections) are randomly ignored (or "discarded").

As shown in Figure 4, by continuously adjusting the neuron parameters in the training of the network, the training set loss size obtained by the final training is 0.060, and the validation set loss size is 0.076.

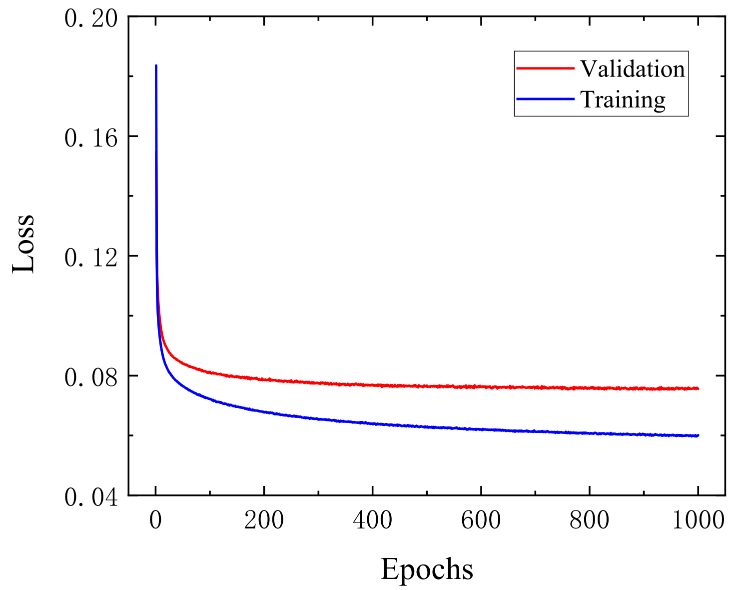

Fig. 4 Inverse network loss function change curve chart

After the reverse network training is completed, the data in the test set is input into the previously trained forward prediction neural network through the structural parameters predicted by the reverse network to obtain the predicted spectrum. If the error between the predicted spectrum and the input spectrum is within the expected range, the trained model of the reverse design neural network meets the designed requirements.

3. Network training results and discussion

In order to more systematically demonstrate the superiority of the forward prediction network model in design performance, this paper has selected the data in the test set to evaluate its performance. The core task of the forward network is to predict the spectral response curve corresponding to the structure, and compare and analyze the spectral response results output by it with the actual spectral response. In order to more clearly reflect the training effect of the model, some test results are randomly selected in Figure 5. for display. In the figure, the blue solid line represents the real spectral response curve, while the red dotted line represents the spectral response curve predicted by the forward network. The structure shown corresponds to the actual spectral response curve, where the green area represents metal and the gray area represents air. IL1 and IL2 are divided into the insertion loss of the predicted and actual spectra, where the calculation formula of the insertion loss is $10\lg T$, and T is the transmittance of the center frequency. It can be observed that the two curves have a high degree of fit and the transmission peaks are basically the same, which shows that the forward design network model proposed in this paper can accurately predict the spectral response of the structure. In addition, the network can usually generate output results within milliseconds, which greatly improves the design efficiency and brings significant time advantages to the researchers' work.

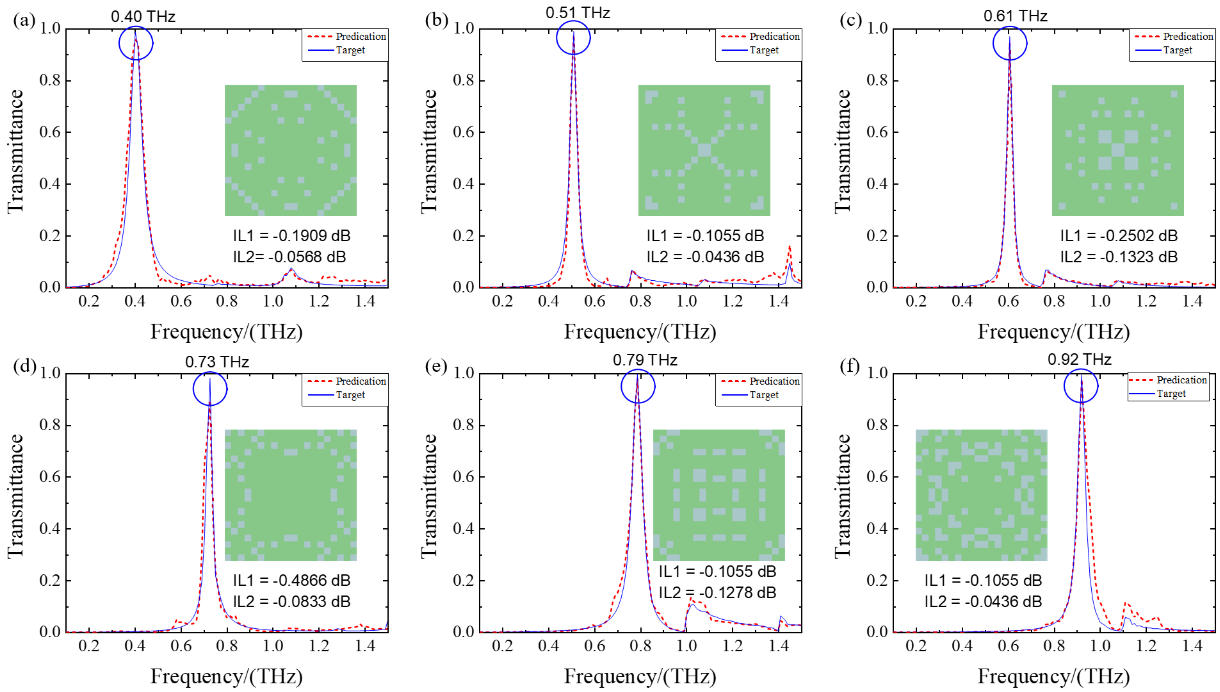

Fig.5 (a-f) Forward network prediction results

In the evaluation of the reverse network model, the data in the test set is also used to verify its effect. The task of the reverse network is to predict the corresponding structural parameters based on the given target spectral response. In order to verify its accuracy, the structural parameters predicted by the reverse network are input into the previously trained forward network to generate the corresponding spectral response, which is then compared and analyzed with the target spectral response to evaluate the accuracy of the reverse network prediction structure. Then some test results are randomly selected, as shown in Figure 6. Among them, the blue solid line represents the target spectral response, and the red dotted line represents the spectral response generated by the predicted structure through the forward network. The structure shown in the figure is the structural parameters predicted by the reverse network.

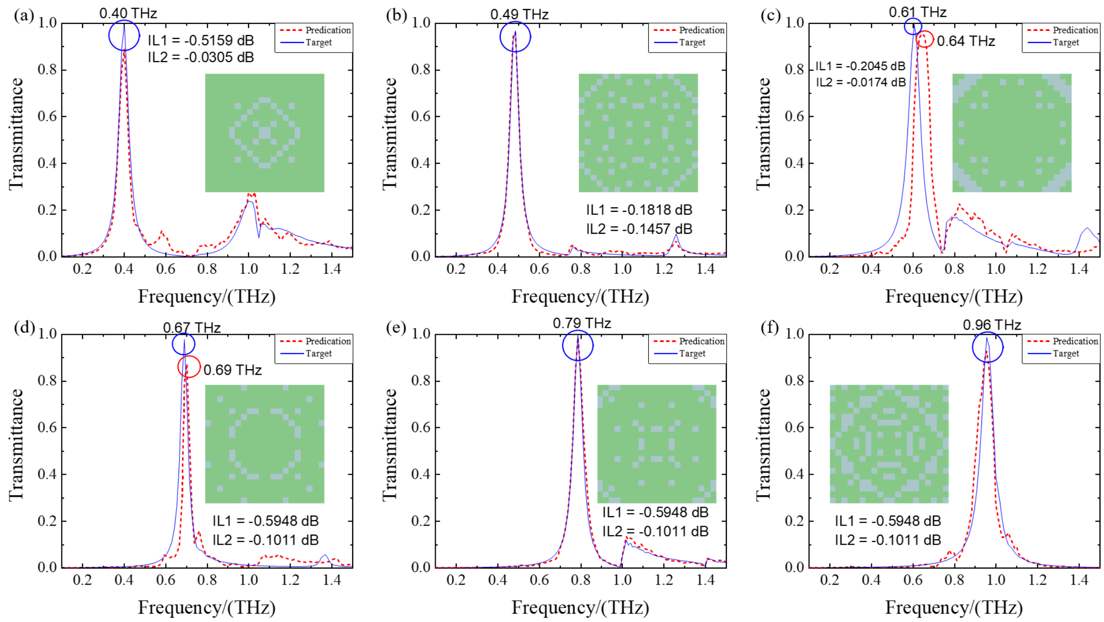

Fig.6 (a-f) Reverse network prediction results

From the results, it can be seen that as shown in Figure 6 (c) and (d), the loss value is larger. Although the transmission spectrum obtained by forward network simulation after the target transmittance curve and the structure output by the reverse design network still has a certain frequency offset in some bands, the overall waveform and center frequency position basically meet the design requirements. This shows that the reverse design network model can accurately and efficiently design a terahertz filter metasurface structure that meets the expectations according to the given target spectrum response parameters and the adjustable center frequency. In this way, the reverse design network demonstrates its potential and practicality in rapidly generating complex electromagnetic structures, proving the advantages and application prospects of deep learning in metasurface design.

In order to further verify the accuracy of the reverse design network model, this paper randomly selects 100 samples from the reverse network test set and inputs them into the forward network. For samples with a large number of frequency offsets and insufficient peak transmittance, this paper identifies such samples as samples with failed predictions. For samples with a small amount of frequency offsets and a small amount of insufficient peak transmittance, but generally meet the design requirements, this paper identifies such samples as samples with successful predictions. Through the statistics of the test set samples, 87 samples out of 100 samples are predicted correctly, and the MSE of these 100 samples is shown in Figure 7. The error composition includes the forward design network and the reverse design network. It can be seen that a small number of samples have a large MSE, but 87% of the samples have an MSE less than 0.005. It can be estimated that the prediction accuracy of the reverse design network model proposed in this paper is about 87%, which further proves the advantages and application prospects of deep learning in metasurface design.

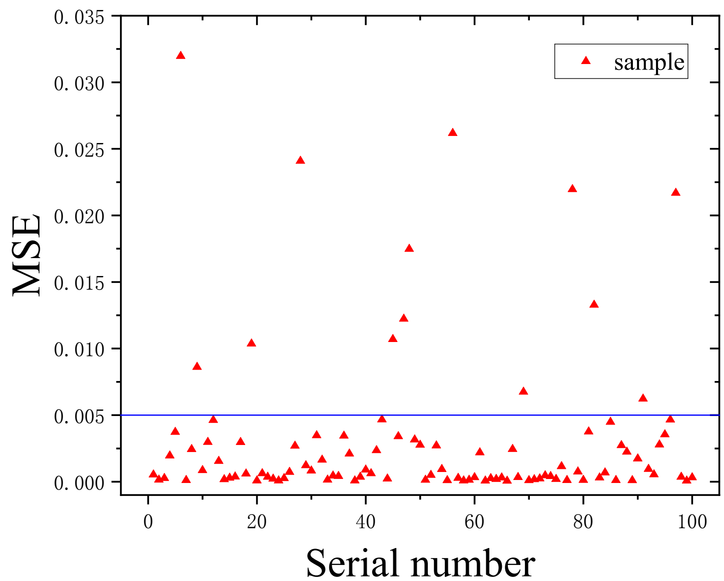

Fig.7 Test set sample MSE distribution

As shown in Figure 8 (b), the structure is iteratively designed through the BPSO algorithm, and the entire BPSO optimization process requires about 11550 seconds of simulation time to complete one optimization [21]. However, in Figure 8 (a), it only takes 30 milliseconds to complete a structural design using deep learning. In contrast, deep learning can not only complete the target structure design at the millisecond level, but also significantly reduce the consumption of computing resources. In addition, the structural performance of deep learning design is equivalent to that of the BPSO method, but the efficiency is significantly superior. Therefore, conducting research on deep learning in terahertz metasurfaces is particularly important for future metasurface designs.

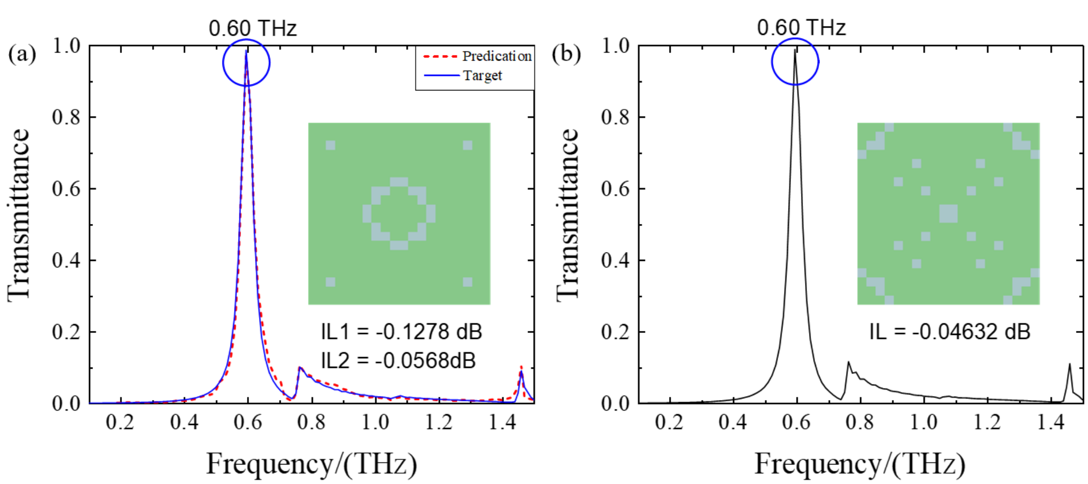

Fig. 8 (a) Convolutional neural network predicted structure and corresponding transmittance; (b) The unit structure and corresponding transmittance curve after BPSO algorithm optimization

4. Conclusions

This paper constructs a forward neural prediction network and a reverse neural prediction network based on the convolutional neural network CNN. The forward prediction network can quickly predict the transmittance curve through the structure. Although it will take a certain amount of time in the process of data set collection and network training, once the network training is completed, the calculation speed will become very fast. Just input the structural parameters into the network, and the spectrum response curve corresponding to the terahertz filter super surface structure can be accurately obtained within milliseconds. Compared with using simulation software to input the corresponding structural parameters to simulate and calculate the spectrum response, the efficiency of the two differs by dozens or hundreds of times, which greatly improves the design efficiency of researchers. At the same time, the reverse design network can also effectively predict the structural parameters corresponding to the target spectrum response to a certain extent, greatly reducing the design time of the super surface, which also opens up new research methods and approaches for the design of super surface filters.

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