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Research on the Design and Optimization of Photonic Crystal Structures Based on Neural Networks

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ABSTRACT

With the continuous development of photonic crystal structure design, It is extremely difficult to establish an analytical model based on the basic principles of physics and to calculate and solve the appropriate structure to achieve specific photonic properties.Especially when the geometric shape and spatial distribution of the structure are very complex, it is almost impossible to start.The electromagnetic modeling based on numerical simulation method is adopted,Designers also tend to constantly fine-tune the geometry and repeatedly perform simulations to get closer to the target, Relies on past experience in designing templates and takes a long time.Therefore, the reverse design algorithm based on deep learning is used through data-driven modeling. The neural network is used to learn a large amount of data to obtain the corresponding law between the optical characteristics and the design parameters,It can help designers find non-intuitive and irregular photonic crystal structures more effectively.And is beneficial to that refine development of the photonic crystal design.The Artificial neural network model of two-dimensional GaAs photonic crystal point defect microcavity is established to predict the radius of the microcavity. And can provide a rapid design method for subsequent photonic crystal structure research.

KEYWORDS

Photonic crystal; Deep learning; Inverse design; Neural network

1 Introduction

Photonic crystals (PCs) are artificial periodic dielectric structures with photonic band gap (PBG) properties, which can be used in optical communications, biochemical detection,Solar energy collection and quantum information processing have played an important role.People can control the movement of photons by designing and manufacturing photonic crystals and their devices. So as to design the photonic crystal with specific optical properties. However, with the continuous development of photonic crystal structure design,There are more detailed requirements for the characteristics and functions of photonic crystals in practical applications.However, the traditional method based on the basic principles of physics and electromagnetic modeling is very important to find a suitable structure to achieve specific optical characteristics.The research efficiency is low, it is difficult to find a suitable research entry point, and the research takes a long time.Therefore, it has become an urgent need to design photonic crystal structures with high efficiency.In practical application scenarios, the structural design parameters are often inversely derived for photonic crystals with given photonic properties.Therefore, how to quickly design photonic crystals with specific optical properties has become an urgent problem.

Artificial neural network can automatically learn the complex nonlinear mapping relationship from a large number of data.Therefore, as a powerful mechanical learning tool, it is widely used in image recognition, speech recognition and other fields.Remarkable results have been achieved. With the further development of artificial neural network to more disciplines,It also opens up a new direction for the rapid design of micro-photonic devices.For example, Liu et al. Used the network design model based on deep learning to customize the metasurface of optical design through reverse design in 2018.The possibility of using artificial neural networks to design photonic devices is revealed.The research on quantum dot single photon source has aroused more and more interest in the study of photonic crystal microcavities.Among them, two-dimensional photonic crystal microcavity structures with periodically arranged air holes have attracted much attention.Because the structure can be easily obtained on a semiconductor material through electron beam exposure and dry etching processes, the structure has good application scenarios, But it is a difficult and time-consuming task to calculate and inverse design a specific photonic crystal with optical trap power use conventional methods,Therefore, it is of great significance to use the inverse design algorithm based on deep learning to study the design technology of photonic crystal structure.

Plane Wave Expansion (PWE) and Finite-Difference Time-Domain (FDTD), which have been developed in recent years, are effective numerical methods.It has been widely used in the design and analysis of optical waveguide devices.However, these two methods require a very large amount of calculation, and usually require the traversal calculation of the design parameters.The calculation time depends on the size, structure and accuracy of the device.In order to solve the problems of long preparation period and high maintenance cost of the electron beam etching and ultraviolet light etching process of the photonic crystal, The design needs to be optimized before preparation to reduce the trial-and-error cost, Introducing a neural network and taking a photonic crystal microcavity (defect) as a target parameter of the neural network, The artificial neural network is trained by the photonic crystal band data calculated by the PWE algorithm, Thereby obtaining a mathematical model of the relationship between the photonic crystal band data and the size of the microcavity,Can realize that that correspond photonic crystal band data can be obtained by input the specific microcavity size through rapid simulation calculation,It provides a reference for future research in the field of photonic crystal nano-design.

2 .Photonic crystal structure design and modeling process

In the practical application of the etching process, the resonant mode shift is obtained mainly by adjusting the etching parameters,Ideally, in order to make the single quantum dot strongly coupled with the resonant mode, the quantum dot should be located at the maximum field strength of the resonant mode.And the emission wavelength of the quantum dot is consistent with the resonant mode wavelength.However, once the growth of the material is completed, the emission wavelength of the quantum dots generally does not change.Therefore, this paper mainly discusses how to realize the alignment of the resonance mode and the quantum dot on the luminescent spectral line by adjusting the etching process. According to the Maxwell equation, the size of the resonant mode can be adjusted by changing the size of the photonic crystal.Generally, three adjustable parameters are R/a, lattice constant a and the thickness t of the slab waveguide layer. This paper mainly discusses how to adjust the wavelength of the resonant mode by changing the value of R/a.

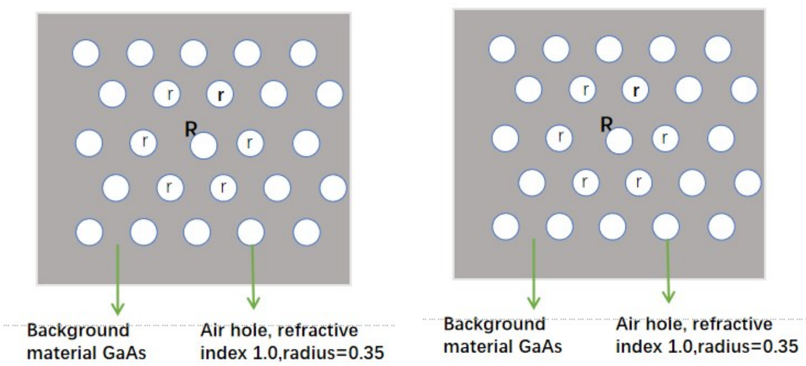

Figure 1 Schematic diagram of two-dimensional GaAs medium background photonic crystal point defect microcavity structure

Figure 1 is a structural schematic diagram of a two-dimensional GaAs medium background photonic crystal point defect microcavity, and the radius of the microcavity is R = 0.02: 0.02: 0.5.The sample data is formed after the photon energy band (dispersion relation ω-K) is calculated by MPB, and then the corresponding neural network is established. Using the photonic crystal model based on neural network, the microcavity radius required for specific band characteristics can be predicted.

3 Calculate the band structure of photonic crystal

The periodic dielectric structure of the photonic crystal forms a photonic band gap through energy band regulation, so that light with a specific frequency cannot be transmitted,Similar to the principle that electrons in semiconductors are limited by energy bands, photonic crystals can be integrated in optical fiber communication devices and systems.Pecially in the aspect of the ultra-small laser array.In that practical design and application of the photonic crystal, the defect structure is often introduce to adjust and control the energy band characteristics of the photonic crystal,Therefore, this study uses the band structure calculated by MPB as the original data set.

As shown in Figure 2, the photonic crystal with two-dimensional air holes arranged in a triangular array under the medium background has the characteristics of multiple band gaps,The shaded area shows one of the band gaps.

Figure 3 shows the energy band characteristics of photonic crystal microcavities with two-dimensional air holes arranged in a triangular lattice under a medium background. Wherein the 50th energy band is a defect mode (or a resonant mode, resonant frequency) located in the first band gap, By comparison, it can be found that the band characteristics of photonic crystals are more complex after the introduction of defect structures.Therefore, in this case, it is difficult to calculate the band characteristics and design the corresponding photonic crystal structure by using the traditional method.Therefore, in this study, the artificial neural network is introduced to build a mathematical model of the relationship between the photonic crystal band data and the size of the microcavity.Help researchers with structural design.

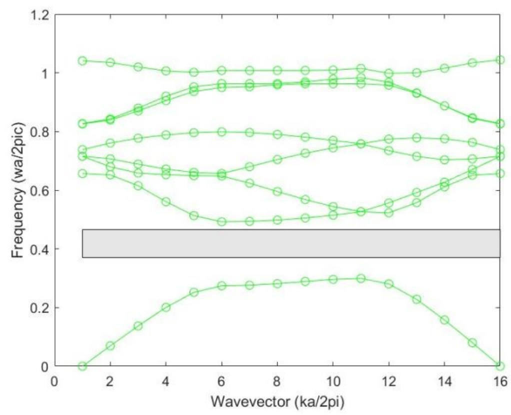

Figure 2 Photonic Crystal Energy Band Characteristics (Defect Free)

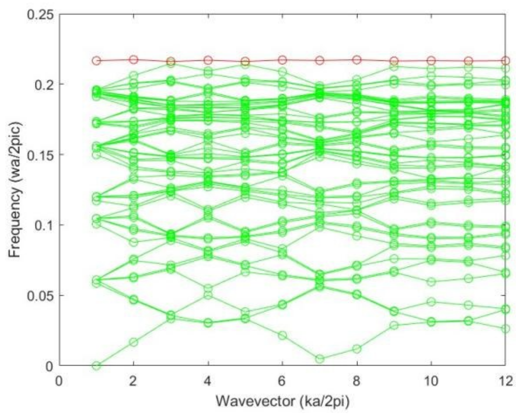

Figure 3 Photonic Crystal Energy Band Characteristics (with Microcavity)

The band structure of two-dimensional GaAs photonic crystal point defect microcavity is calculated by using MPB.

Figure 4 utilizes the MPB (MIT Photon) in the Linux system in the VM virtual machinelcBands) software calculates the energy band data under different defect structures (changing the radius R of the photonic crystal microcavity: 0.01: 0.01: 0.5), And obtaining the intrinsic electromagnetic field frequency Omega and other related electromagnetic field distribution information in the TE/TM mode at different K points.

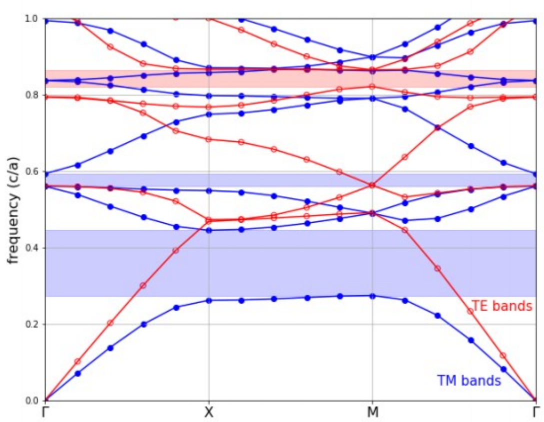

Figure 4 The intrinsic electromagnetic field frequencies of TE/TM modes at different k points in photonic crystals

Use MATLAB to make data set

Because the data set calculated by using MPB software has text information which cannot be directly recognized, Therefore, the relevant code should be compiled to remove the NaN line for data set purification, and finally output the data set for artificial neural network training.

4 Neural network model training and testing

4.1 Generate a training set and a test set

In order to ensure that the established model has good generalization ability, the number of samples in the training set is required to be large enough and have good representativeness.It is generally believed that the number of samples in the training set should account for 2/3-3/4 of the total number of samples, and the remaining 1/4-1/3 should be used as test samples.At the same time, the distribution of training samples and test samples is almost the same.

4.2 Create and train neural networks

Before creating a BP neural network, the structure of the network needs to be determined, that is, the following parameters need to be determined: the number of input variables,The number of hidden layers, the number of neurons in each layer, and the number of output variables.In fact, the three-layer BP neural network with only one hidden layer can approximate any nonlinear function.Therefore, this project only discusses the BP neural network with single hidden layer. As shown in Figure 5, there are 612 nodes (neurons) in the input layer, 9 nodes in the hidden layer, and one node in the output layer.A sigmoid function is used as the activation function for the output of the hidden layer node, and a linear function is used as the activation function for the output layer node. After the network structure is determined, the relevant training parameters (such as training times, learning rate, etc.) Are set, and the network can be trained.

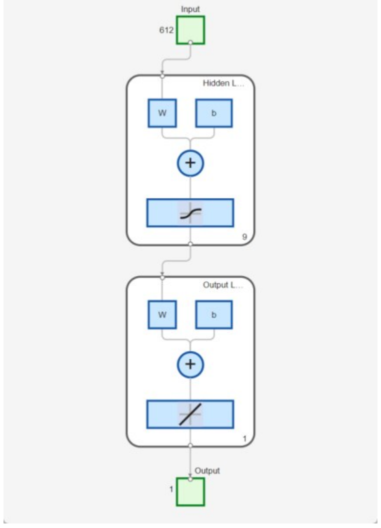

Figure 5 Neural Network Structure

4.3 Simulation test

As shown in Figure 6, after the model training is completed, the input variables of the test set are input into the model. The output of the model is the corresponding prediction result.

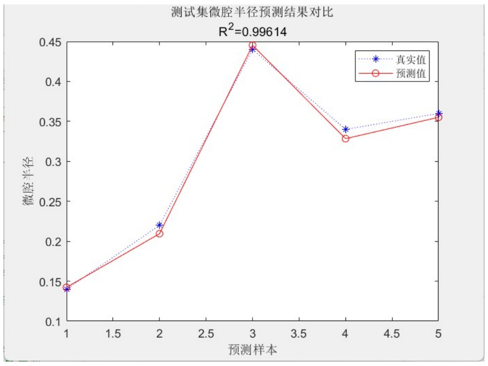

Figure 6 Microcavity Radius Prediction Results

As shown in the figure, the model calculation value of 5 test samples is compared with the actual value, and the correlation coefficient reaches 0.996.It shows that the model has good generalization performance. The simulation test is repeated to obtain that the correlation coefficient is stabilized above 0.99,It can be seen that the neural network model is more in line with the energy band data of two-dimensional GaAs medium background photonic crystal point defect microcavity.The microcavity radius corresponding to the test band data can be well predicted.

4.4 Performance evaluation

BP algorithm is composed of two parts: the forward transmission of information and the backward transmission of error. In the process of forward transmission,The input information is transmitted from the input layer to the output layer through the hidden layer.The state of each layer of neurons only affects the state of the next layer.If the desired output is not obtained at the output layer, the error change value of the output layer is calculated, and then the back propagation is turned. Through the network, the error signal is transmitted back along the original connection path to modify the weights of neurons in each layer until the desired goal is achieved.

By calculating the error between the predicted value A of the test set and the true value (expected value T), the sum of squared errors Σ (n) is minimized.It is approached gradually by continuously computing changes in network weights and biases in the direction of decreasing slope with respect to the error function.Of the target.The changes of weights and biases are proportional to the effects of network errors, and are transmitted to each layer in a backpropagation manner. The Generalization ability of the model can be evaluated.The number of nodes and the size of the weight matrix of the input layer/hidden layer can be optimized to improve the generalization performance of the BP neural network.

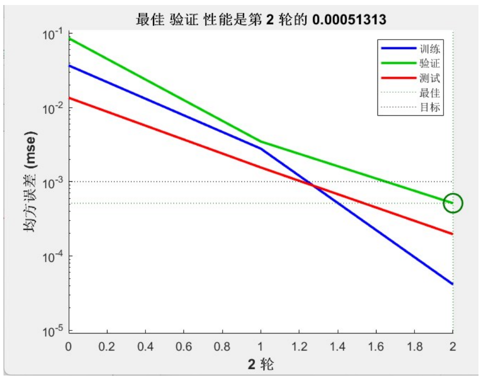

Figure 7 Mean Square Error as a Function of Round Number

Figure 7 shows the change of the mean square error with the number of training rounds, and the model training goal is achieved in the second round of training.Repeated tests show that the model can basically achieve the training goal in 2-6 rounds, and the error of the validation set is stable and there is no overfitting. It can basically complete the use requirements of the model, and then set a reasonable MSE threshold according to the task requirements and data distribution.At the same time, the error of validation set was monitored to further verify the generalization ability.

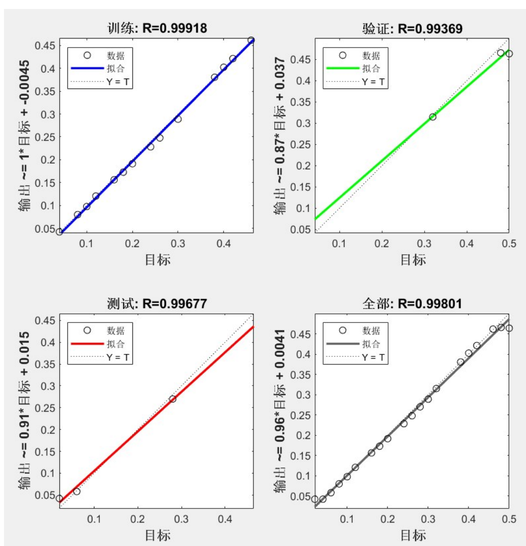

Figure 8 The correlation coefficient between calculated values and actual values

The figure shows the correlation coefficient between the model calculation value and the actual value.The correlation coefficient of the training set is 0.999, and the correlation coefficient of all data sets is 0.998, which indicates that the training data set is acceptable and the model training effect is good.Parameters such as model target setting and learning rate can be adjusted subsequently according to actual needs.

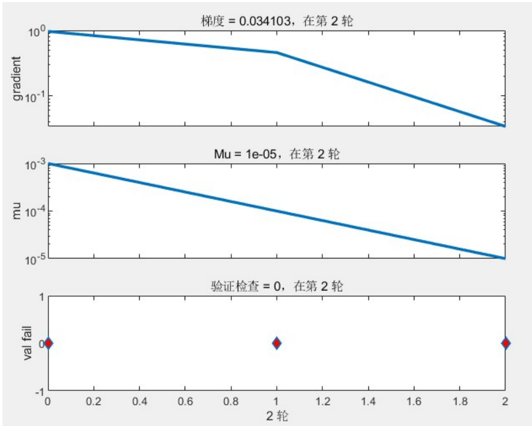

Figure 9 Gradient as a Function of Training Rounds

As shown in the figure, the gradient changes with the number of training rounds, and the gradient drops to the training target in the second round.Repeated tests show that the model can basically achieve the training goal within 2-6 rounds, and can basically complete the use requirements of the model.Subsequently, through gradient monitoring and super-parameter optimization, the convergence speed and model performance can be balanced, and the loss of validation set can be monitored.If it decreases synchronously with the training loss, it is normal;If the validation loss increases, add regularization (such as Dropout, L2) or expand the data set to ensure the generalization of the model.

5 Concluding remarks

This study aims at the problem that specific photonic crystals have complex geometric shapes and spatial distributions. The optical reverse design technology of photonic crystal based on deep learning is used to speed up the performance prediction of photonic crystal.So that people can find non-intuitive and irregular photonic crystal structures,It can provide a reference for future research in the field of photonic crystal nano-design.

In this study, BP neural network is used to establish the relationship between the band data of two-dimensional GaAs photonic crystal point defect microcavity and the size of the microcavity.Learning model solves the problems of low research efficiency and long research and development time of traditional modeling methods.For the field of photonic crystal design and fabrication, it is expected that an efficient photonic crystal reverse design technique can be provided, Improve the design speed and desired accuracy of photonic crystals.Future work will focus on using more accurate training strategies to ensure the accuracy of the model's predicted optical performance.Optimize the reverse design of complex geometric structures, and try to further improve the generalization ability of the model.

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