ISSN 2959-6157

A neural network model for point defect microcavities of two-dimensional GaAs media background photonic crystals

Lihao Fan

College of Computer and Cyber Security, Fujian Normal University, Fuzhou, Fujian, 350117, China
121152021078@student.fjnu.edu.cn

Abstract:

This paper aims to address the challenge of constructing, training, and optimizing a neural network model for the point defect microcavity of a two-dimensional GaAs media background photonic crystal. The objective is to achieve more accurate predictions and analyses of photon modes, thereby enhancing the performance of the microcavity. Due to the structural complexity and multi-parameter nature of point defect microcavities, traditional analysis methods often fail to capture their optical behavior adequately. Consequently, there is a need for a novel approach to establishing an optical model for point defect microcavities, enabling precise predictions of their optical properties and optimal design. In this study, the MPB computing tool developed by MIT, in conjunction with the programming language Scheme, MATLAB, and the Ubuntu virtual machine platform, was utilized for data acquisition. The neural network model was employed to process the input data of the photonic crystal point defect microcavity, leading to predictions and analyses. This interdisciplinary approach results in a high-precision model of the microcavity. The neural network model is capable of nonlinear mapping and prediction by learning the patterns and features of the data. Additionally, this combination holds the promise of enabling more efficient optical information processing and increased data transfer rates. The relationship between the energy band data and the structure of photonic crystals exhibits a high degree of nonlinearity. The neural network model proposed in this paper can infer the structure of photonic crystals based on the photon energy band (dispersion relation ω-K) of micro-cavity structures with point defects in different photonic crystals. This provides a valuable reference for more accurate predictions and analyses of photon modes in complex photonic crystal micro-cavities, ultimately leading to improved micro-cavity performance.

Keywords: Two-dimensional photonic crystals, Point defect microcavities, Neural networks, Dispersion relation, Optical model prediction

1. Introduction

1.1 *Research Background and significance*

Gallium arsenide (GaAs) is a common semiconductor material. It has good optical and electronic properties, so it is often used as a material for the manufacture of various optoelectronic devices and satellite communications. These properties of gallium arsenide make it an ideal dielectric background for photonic crystals. A photonic crystal is a material with a periodic refractive index that prohibits the propagation of electromagnetic waves in certain frequency ranges, creating a so-called photonic band gap. We introduce local defects in photonic crystals, which can cause local modes to appear in photonic band gaps and form micro-optical cavities.[1]

Because of its superior physical properties and highly adjustable design freedom, photonic crystal microcavities have attracted a large number of researchers for in-depth research. Among them, theoretical models of such microcavities are crucial for understanding and predicting experimental results. However, such models often require complex computational processes and deal with a large number of parameters, making it a challenge to accurately describe and optimize them.

In recent years, neural networks, as a powerful machine learning technique, have been widely used in the modelling and optimization of various complex systems. By using a set of photonic crystal band structure calculation tools MPB and Scheme programming language developed by MIT researchers to collect data and then train neural networks, it is possible to achieve efficient and accurate modelling of complex systems. Point-defect microcavities are localized structures in two-dimensional GaAs dielectric background photonic crystals, which have the ability to modulate optical modes and enhance light-matter interactions. The neural network model is used to study and optimize the optical properties of the point defect microcavity. By learning and training the relationship between the input and output, the optical properties of the point defect microcavity can be predicted quickly and accurately, which can effectively solve the structural complexity and multi-parameter characteristics of the defect microcavity faced by the traditional method in the design and optimization of the point defect microcavity. To achieve accurate prediction and optimal design of its optical properties, promote the development of photonic devices and photonic integration technology. Therefore, the application of neural network to the model construction of point defect microcavity of two-dimensional GaAs media background photonic crystal is not only an attempt to the application of neural network in the field of physics but also to solve the problem that the traditional model is difficult to deal with.

The neural network model of point defect microcavity of two-dimensional GaAs photonic crystals is an advanced research topic integrating semiconductor physics, optoelectronics and artificial intelligence. From a macro point of view, with the increasing demand for efficient, low-energy and miniaturized equipment in society, the development of high-performance optoelectronic equipment has become an urgent need. However, the control and processing of optical signals by using two-dimensional GaAs background photonic crystal point defect microcavity is an important research content in this direction. At the same time, the introduction of neural network model can improve the intelligence of the equipment, further optimize the calculation process, and improve the accuracy. Furthermore, it can effectively solve the problems faced by traditional methods in the design and optimization of point-defect microcavities, such as high design complexity, difficult regulation, difficult system integration, and high preparation accuracy requirements. It will promote the development of photonic devices and photonic integration technology, and promote the development of photonics in future communication, information processing, sensing and other fields, which have great application potential and theoretical significance.

1.2 *Related work*

Zhong Xianghui used the finite element method to numerically simulate two-dimensional photonic crystal microcavity and optimized the performance of the microcavity by adjusting the structural parameters of the microcavity [2]. At the same time, he also carried out simulation research on two-dimensional photonic crystal microcavities containing dispersive media, which provided a certain theoretical significance for the preparation of photonic crystal microcavities in the future. V. Vita et al. have successfully studied the photonic band gap of two-dimensional photonic crystals and found that the band gap can be controlled by changing the properties of the scatterers, which provides an important theoretical basis for further research and application of photonic crystals [3]. Peichen Yu et al. described the spontaneous emission characteristics of self-organized InAs/GaAs quantum dots in photonic crystal microcavities, successfully demonstrated the feasibility of using photonic crystals to fabricate optical microcavities and control the spontaneous emission both theoretically and practically, and fabricated a novel electro injection surface emission photonic crystal microcavity [4]. Between 2017 and 2020, the MIT research team achieved efficient single-photon emission using point-defect microcavities in two-dimensional materials. They successfully fabricated 3D photonic crystal structures with high-quality factors using advanced nanofanufacturing techniques, and studied their optical properties and regulatory mechanisms. Their research results provide an important foundation for the application of photonic crystals in optical sensing, photonic integrated circuits and quantum optics, demonstrating the importance of point-defect microcavities in quantum optics and photonics applications. A team at the University of Cambridge in the UK has made an important breakthrough in the study of photonic crystal microcavities. They used fiber taper technology and atomic layer deposition technology to fabricate photonic crystal microcavities with highly strong coupling, and realized the manipulation of single quantum dots and the control of quantum states. Their research results provide new platforms and tools for the development of fields such as quantum communication and quantum computing.

The neural network model of point defect microcavity in two-dimensional GaAs background photonic crystal can be interpreted by referring to the deep learning theory (LeCun, Bengio, & Hinton, 2015) [5]. Deep learning theory points out that artificial neural networks can learn by themselves and gradually optimize the accuracy of prediction or classification by simulating the connections between neurons and information processing in the human brain. And as the number of layers (i.e., "depth") of a neural network increases, so does its ability to handle complex problems.

According to this theory, we can consider that the point defect microcavity of 2D GaAs dielectric background photonic crystal has a certain "depth", so it can be simulated by neural network. Such a model would have the ability to learn and optimize itself and be able to describe the behavior and properties of the microcavity more precisely.

The main impact of this model on photonic crystal point defect microcavities is to provide a new and effective analytical tool that can improve our understanding and control of such microcavities. At the same time, by training the neural network, we may also be able to discover some unknown microcavity behaviors and properties.

The above proposed mechanism has been verified in other physical systems. For example, neural networks have been successfully applied to simulate and predict the behavior of quantum systems [6] (Carleo & Troyer, 2017). However, this method has not been widely used in the study of point-defect microcavities in photonic crystals, and my study may fill this gap.

2. Materials and Methods

2.1 *Data acquisition and preprocessing*

First, the Ubuntu virtual machine was used to build the MIT open source model. This model is calculated using the Scheme programming language and MPB, which can provide us with the photon energy bands (dispersion relation ω-K) of different photonic crystal microcavity structures with point defects. In this stage, we want to ensure the correctness and stability of the model in order to produce high-quality raw data. Since the quality of the data directly affects the subsequent training of the model, a lot of effort needs to be invested in optimizing and debugging the model to operate stably under various parameter Settings with as little error as possible.

Next, the collected sample data are thoroughly preprocessed, including steps such as data cleaning, denoising and normalization. In the data cleaning phase, we need to remove invalid or erroneous data such as values out of the expected range, duplicate data, etc. In the denoising stage, we will use various statistical methods and machine learning algorithms, such as filters, principal component analysis, etc., to remove noise from the data. Finally, in the normalization phase, we will transform the data into a format that is easier to work with, for example, by mapping all the data to a scale of 0 to 1, or by making each feature have a mean of 0 and a standard deviation of 1. These preprocessing steps can greatly improve the efficiency and accuracy of subsequent model training.

In order to simulate the characteristics of the photonic crystal and explore the influence of the radius of the gas cylinder on the band structure of the photonic crystal. I did this by varying the radius of the cylinder (from 0.01 to 0.51) and seeing how this change affects the band structure of the TE mode. I used Meep library, an open source finite difference time domain (FDTD) electromagnetic simulation package, whose main interface language is Scheme. In this way, researchers can describe physical problems in a more high-level and intuitive language without having to care about the underlying computational details.

A 5x5 2D geometric grid is first defined with basis vectors (sqrt(3)/2, 0.5) and (sqrt(3)/2, -0.5), and the default material is set to a dielectric constant of 12. Define a gas cylinder (radius 0.2, infinite height) at the center of the grid. Copying this cylinder to the entire grid forms a photonic crystal structure. Gas cylinders with radii varying from 0.01 to 0.51 were then successively added to the existing photonic crystal structure through a cycle. Set the spatial resolution to 16 pixels/unit length and the number of bands you want to compute to 10. Two k points are defined: Gamma point (the center of the Brillouin zone) and K' point (the edge of the Brillouin zone). Then 10 K points obtained by interpolation between Gamma point and K' point are set. And at the end of each loop, print the radius r of the current cylinder.

2.2 *Dataset Partitioning and model training*

Photonic crystal simulation result data is read in MATLAB (stored in virtual machine ". dat "file) and then processed and saved to obtain a sample dataset. According to the characteristics of the point defect microcavity of photonic crystal in 2D GaAs medium background, we will design BP neural network for data modeling and prediction. Load the data from the previously saved "dataset.mat" file and copy it 100 times. The replicated data is then divided into two parts, one for training the Ann and the other for testing the performance of the Ann. The first 4950 rows of the replicated dataset are then selected as the training set, where all columns (except the last column) are used as input features and the last column is used as the target value. The remaining rows of the replicated dataset are selected as the test set, and the size of the test set is calculated. A new feedforward neural network is created with the input layer corresponding to the features of the training set, the output layer corresponding to the target value of the training set, and the hidden layer with 9 neurons. The training parameters of the neural network were set, including the number of training rounds (1000 times), the target error (1e-3), and the learning rate (0.01). The neural network is then trained using the training set. Finally, the trained neural network is used to predict the test set.

2.3 *Validation and tuning*

The training of neural networks requires a lot of data. The current experimental technology has been able to provide enough experimental data, including the optical characteristics of the photonic crystal microcavity under different materials, different structures and different process conditions. In addition, a large amount of simulation data can be generated through theoretical calculation and simulation. These data provide the possibility for the training of neural networks.

Next, the performance evaluation is carried out to calculate the relative error and the coefficient of determination R^2 to evaluate the prediction performance of the neural network. And put the prediction result, the actual value and the error into a matrix. The last section is a plot showing the actual versus predicted values and the coefficient of determination, R^2. The validation set is used to evaluate the performance of the trained model, and the model parameters, such as network architecture, learning rate, and batch size, are adjusted according to the evaluation results. We will iterate this process until a satisfactory performance metric is reached.

2.4 *Model testing*

Although the behavior of photonic crystal microcavities is very complex, theoretical studies have shown that neural networks are capable of handling this complexity. Specifically, some theories prove that neural networks can approximate any complex function with arbitrary precision, which provides theoretical assurance for neural networks to handle the complex behavior of photonic crystal microcavities. For example, the theoretical study of Cybenko (1989) proved the approximation ability of neural networks[7]. Finally an independent test set is used to evaluate the performance of the optimized model on unseen data. Through the analysis of the test results, we can further understand the stability, reliability, and generalization ability of the model.

3. Results and discussions

k (kx, ky, kz) and w (angular frequency) are successively extracted using the instructions of MPB software. After obtaining k and w, the energy band diagram (denoted by red and o) is plotted. The horizontal axis represents certain directions of the Brillouin zone, where the points Y, Gama, and X, M are points in several special inverted lattice Spaces. While the vertical axis is the frequency of the electromagnetic wave. In the figure, there are structures representing the TM wave band and the TE wave band. Two-dimensional photonic crystals, for example, are usually binary media composed of many dielectric columns or holes. If we consider the total electromagnetic field in the medium, the electromagnetic fields at the boundary of these cylinders must be connected in a way that satisfies the boundary conditions. When there are infinitely many cylinders, there are infinitely many boundary conditions that must be satisfied, and if the boundary conditions cannot be satisfied for any waveform within a full frequency range, the frequency is the band gap.

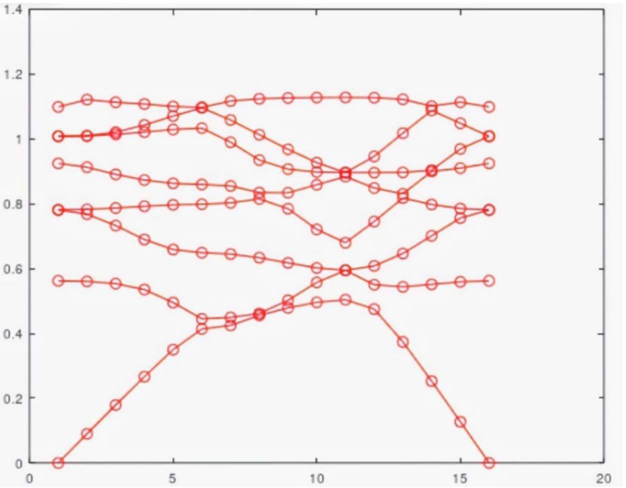

Figure 1. Photonic crystal band structure diagram

There is no linear relationship between photonic crystal band data and structure, but it is highly nonlinear and discrete. In this study, the relationship between the radius of the point defect microcavity and the photon energy band is expressed by the neural network model, and a special energy band relationship is found, and the neural network is good at establishing the nonlinear relationship model between two variables. In the background of GaAs, after the neural network model is established by periodic arrangement of air holes, the size and structure of the photonic crystal microcavity need to be inverted by the frequency of the microcavity with point defects.

Once the neural network is up and running, we get a comparison plot of the predictions for the test set.

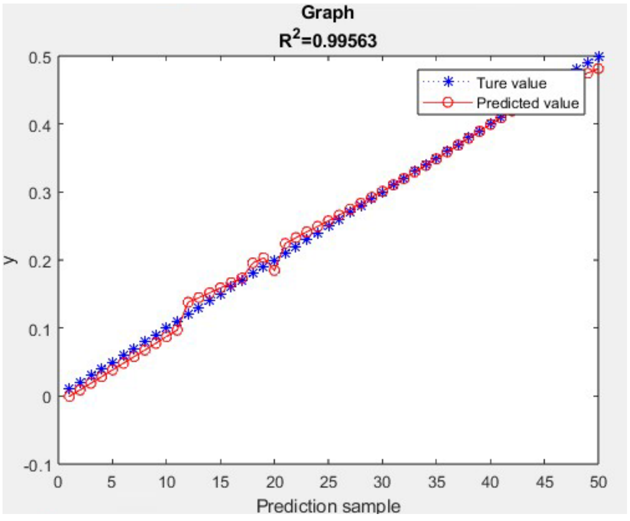

Figure 2. Comparison of test set prediction results

Opening the neural network view, the input layer has 121 nodes, the hidden layer has 9 nodes, and the output layer has only 1 node.

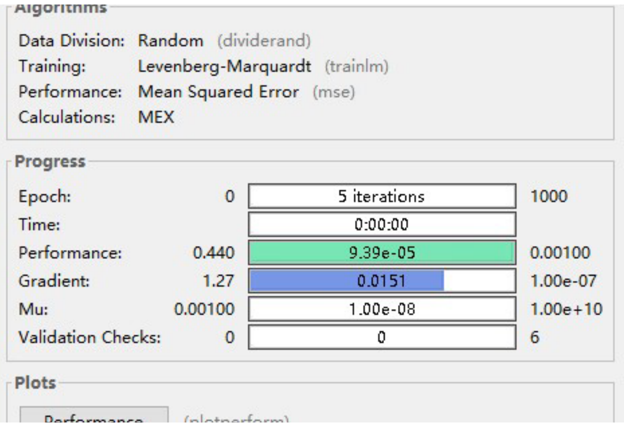

Figure 3. BP neural network simulation diagram

When we open the performance vs. training state graph again, we can see how the number of iterations changed during training. As the number of iterations and training increases, the mean square error is decreasing. Finally, the regression graph is observed, which also confirms the conclusion of this study.

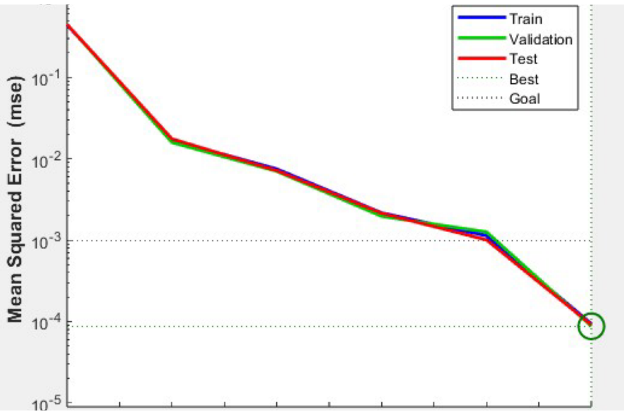

Figure 4. BP neural network training performance diagram

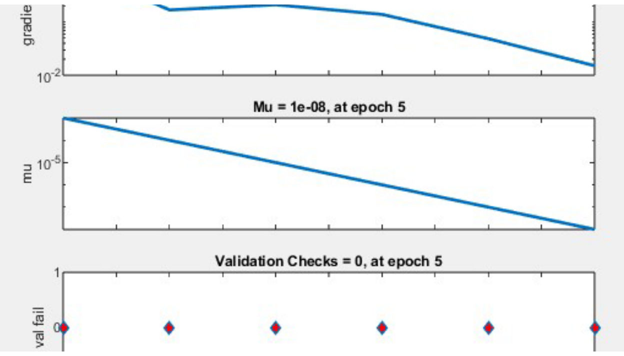

Figure 5. BP neural network test results

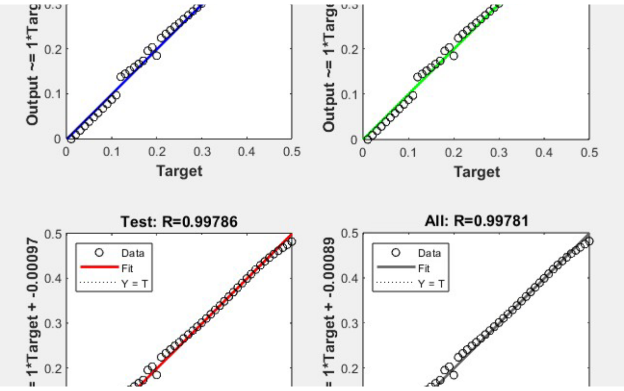

Figure 6. Neural network training regression graph, Epoch 5 achieved optimal performance

4. Conclusion

In this study, we used a backpropagation neural network model to characterize and predict the characteristics of point defect microcavities of two-dimensional GaAs background photonic crystals. We first obtain the relationship between the microcavity radius and its photon band through a large number of simulation experiments, and input these data into the neural network model as a training set and a test set.

After proper training and optimization, the model can effectively predict the photon mode at a given microcavity radius. In addition, the size and structure of the photonic crystal microcavity are also deduced successfully by using the frequency of the point defect microcavity.

This result is of great value for further understanding of the photon mode of the photonic crystal microcavity and its relationship with the structural parameters of the microcavity. The prediction results of neural network model can provide important reference for the design and optimization of photonic crystal structure, so as to improve the optical performance of microcavity. In the future, we will further improve the prediction accuracy of the model in order to more accurately guide the design and preparation of photonic crystal microcavities.

Overall, this study shows that using neural network models to predict the photon patterns of photonic crystal microcavities is a feasible and effective method. We expect that this method can be more widely used in photonic crystal and related fields, and the simulation results can provide some theoretical references for the design of photonic crystal devices, so as to promote the further development of this field.

5. References

[1] Zhang R J. Photonic crystal vertical-cavity surface-emitting lasers and optimized design[J]. Micronanoelectronic Technology,

2006, 43(9): 420-425.
[2] Zhong Xianghui. Finite element simulation and optimization of photonic crystal microcavity [D]. Beijing university of posts and telecommunications, 2022. The DOI: 10.26969 /, dc nki. Gbydu. 2022.001983.
[3] Vinita, Vinita et al. "Impact of geometry on Photonic Bandgaps for TE polarization in two-dimensional Photonic Crystals with triangular lattice." *2013 Students Conference on Engineering and Systems (SCES)* (2013): 1-5.
[4] P. . -C. Yu, J. Sabarinathan, B. Kochman, S. Krishna and P. Bhattacharya, "Enhanced spontaneous emission from InAs self-organized quantum dots in a two-dimensional GaAs photonic crystal defect microcavity," *2002 Summaries of Papers Presented at the Quantum Electronics and Laser Science Conference*, Long Beach, CA, USA, 2002, pp. 59-60, doi: 10.1109/QELS.2002.1031092.
[5] LeCun Y, Bengio Y, Hinton G. Deep learning. Nature. 2015 May 28;521(7553):436-44. doi: 10.1038/nature14539. PMID: 26017442.
[6] Giuseppe Carleo, Matthias Troyer, Solving the quantum many-body problem with artificial neural networks. Science355,602-606(2017).DOI:10.1126/science.aag2302
[7] Cybenko, George V.. "Approximation by superpositions of a sigmoidal function." *Mathematics of Control, Signals and Systems* 2 (1989): 303-314.