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Neural network-based prediction and optimization of optical properties of two-dimensional GaAs dielectric background photonic crystal point-defect microcavities

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Abstract:

The aim of this study is to develop a neural network model of point-defect microcavities in two-dimensional GaAs dielectric background photonic crystals in order to accurately predict and optimize their optical properties. Point-defect microcavities are localized structures in photonic crystals with the ability to modulate optical modes and enhance light-matter interactions. However, existing methods are unable to fully capture their complexity and multiparametric properties. Therefore, present study propose to utilize a neural network model to quickly and accurately predict the optical properties of point-defect microcavities. With this model, present study can effectively address the challenges faced by conventional methods in design and optimization. The results of this study will promote the development of photonic devices and photonic integration technologies, and facilitate the application of photonics in the fields of information technology, communication, energy and biomedicine.

Keywords: photonic crystal, point defect microcavity, neural network model, optimization design

1. Introduction

A photonic crystal is a structure with a special material, proposed by John S. and Yablonovitch E. et al. in 1987. It has a “photonic frequency forbidden band”, i.e., a defect is introduced into a perfect photonic crystal. When the frequency of the electromagnetic wave coincides with the defect state, it may be localized at the defect location. Point-defect microcavities are localized structures in photonic crystals, which form locally modulated optical modes by introducing defects in the lattice. Currently, researchers have studied the optical properties of point-defect microcavities to some extent through theoretical simulations and experimental measurements. However, the relationship between the optical properties and structural parameters of point-defect microcavities is still not completely clear. Conventional methods often require extensive trial-and-error and optimization processes, which are time-consuming and not efficient enough. In addition, due to the structural complexity and multi-parameter characteristics of point-defect microcavities, traditional analytical methods are often unable to fully capture their optical behavior. Therefore, there is a need to find a new method to establish the optical model of point-defect microcavities to achieve accurate prediction of their optical properties and optimized design.

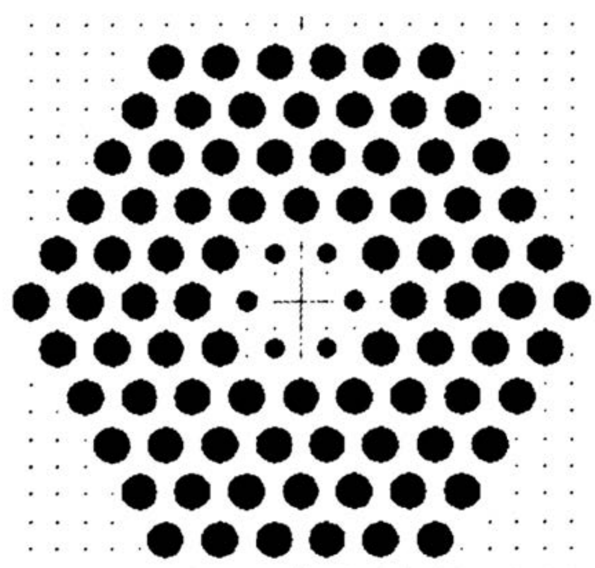

Figure 1 2D triangular lattice band defect structure photonic crystal

In 2019, by a team of scientists from McGill University in Canada, they successfully combined the optical properties of photonic crystals with the computational capabilities of neural networks to realize a photonic crystal neural network chip. The photonic crystal neural network chip is based on the optical nonlinear properties of photonic crystals, and uses the transmission and control of light to realize the computational functions of neural networks. Since photonic crystal is a periodic optical material with a specific refractive index distribution, it can realize the waveguide and modulation of light, while neural network is a computational model that mimics the human nervous system, which is used to process complex data and perform pattern recognition. Combining photonic crystals with neural networks benefits to some extent from the optical properties of photonic crystals and the fast transmission speed of light, as well as the computational and pattern recognition capabilities of neural networks. The combination of the two offers new possibilities for high-speed and efficient optical computation. Compared to traditional optical simulation methods that rely on physical equations and numerical solution methods, the use of neural networks for learning patterns and features of data to achieve nonlinear mapping and prediction has the advantages of simplicity, accuracy, efficiency and universality.

In this study, a neural network model was constructed for a two-dimensional GaAs dielectric background photonic crystal point-defect microcavity, and the model was used to achieve accurate prediction and analysis of photon modes and dispersion relations of the photonic crystal point-defect microcavity.

2. Modeling a photonic crystal point-defect microcavity with a two-dimensional GaAs dielectric background

First, present study selected a lattice size of 5x5 to ensure that the photonic crystal has sufficient size and periodicity. The lattice is defined by two basis vectors, and to meet the geometrical requirements of the structure during the construction of the photonic crystal, present study used GaAs as the default material and set its dielectric constant to (epsilon) 12 to accurately characterize the optical properties of GaAs. In order to introduce point-defect microcavities, present study added cylindrical structures to the lattice. The material of these cylinders was chosen to be air (air) and its radius (r) is a variable parameter. Present study used a sequence of radii ranging from 0.01 to 0.51 in steps of 0.01 to study the effect of different sizes of defective microcavities on the properties of photonic crystals. Such a design allows us to explore the optical response induced by defective microcavities of different sizes in photonic crystals.

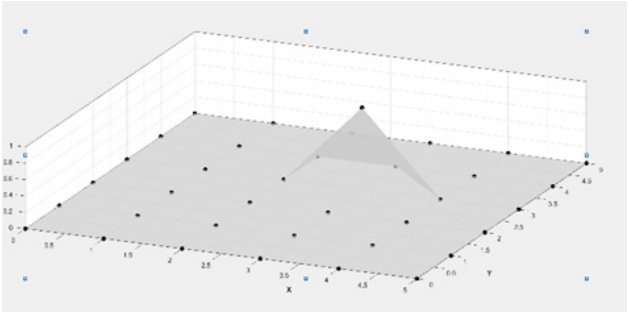

Figure 2 Modeling of photonic crystal point-defect microcavities on a 2D GaAs dielectric background

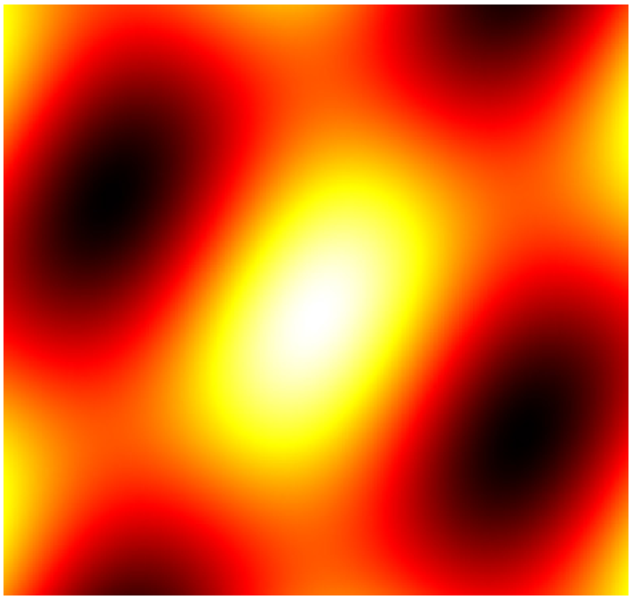

Figure 3 Photonic crystal with GaAs dielectric background

3. Data acquisition

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Figure 4 Sample photonic crystal point-defect microcavity structures with different radii and their corresponding partial photon modes and dispersion relations for a 2D GaAs dielectric background

(1) Iterative Addition of Cylinders: A loop iteration approach was employed to add cylinders with different radii to the list of geometries. Each iteration involved the addition of a cylinder with a specific radius, allowing for the exploration of different sizes of defective microcavities in the photonic crystal.

(2) Setting Simulation Parameters: The simulation parameters were carefully defined to ensure accurate calculations. This included specifying the resolution of the simulation and determining the number of bands to consider in the analysis.

(3) Definition of Key Points: Two crucial points, namely the Γ-point (Gamma) and the K'-point (K'), were defined. These points serve as reference positions in the analysis of the photonic crystal's energy band structure.

(4) Generation of K-Points: A series of K-points, totaling ten in number, were generated between the Γ-point and the K'-point. These K-points are strategically positioned to capture important characteristics of the photonic crystal's energy bands.

(5) Energy Band Calculation: The energy band structure of the photonic crystal was calculated using the energy band calculation method (run-te). This calculation involved considering the defined geometries, simulation parameters, and the generated K-points. The resulting energy band structure provides valuable insights into the behavior of the photonic crystal.

(6) Recording of Radius Values: During the iteration process, the current value of the radius (r) was recorded for each iteration. This allowed for the generation of a sequence of radii ranging from 0.01 to 0.51 with a step size of 0.01. By systematically varying the radius, the influence of different sizes of defective microcavities on the properties of the photonic crystal could be examined.

In short present study build a photonic crystal point-defect microcavity model with a two-dimensional GaAs dielectric background and explore the energy band structure of photonic crystals by cyclically adding cylindrical defects of different radii. By modifying the radius sequence and simulation parameters, sample data of the energy bands (dispersion relation ω-K) of photonic crystals can be obtained for defects of different sizes.

4. Designing, training neural network models

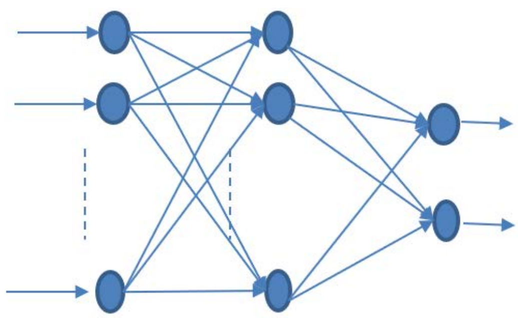

Figure 5 Model structure framework

(1) set/test set generation: sample data from the energy bands of photonic crystals are used and copied several times to increase the number of samples. The dataset is then divided into a training set and a test set.

(2) BP Neural Network Creation, Training and Simulation Testing:

a. Network Creation: create a new neural network object using the selected neural network model (BP neural network). Set the size of the input layer to the number of features in the dataset, the size of the output layer to the number of target variables, and select the appropriate hidden layer size.

BP neural network creation:

a. A new neural network object was created using the newff (Feedforward Neural Network) function. The input parameters of this function include the input features of the training set (P_train) and the target output (T train), as well as a parameter indicating the structure of the hidden layer, which is 9 here.

b. Setting training parameters: set the training parameters of the neural network, including the number of iterations (epochs), the target error (goal) and the learning rate (lr). These parameters will affect the training process and results of the network.

c. Training the network: the neural network is trained using the input features and target output of the training set. During the training process, the neural network is adjusted to its internal weights and biases to minimize the error between the predicted output and the target output. The training process is iterated several times until a specified number of iterations or target error is reached.

d. Simulation test: the trained neural network is used to simulate the input features of the test set to get the predicted target output. Here the variable T sim bp is the prediction obtained by simulation test through neural network.

Performance evaluation: the performance of the model is evaluated based on the results of the simulation tests. Two performance evaluation metrics are used here:

a. Relative error (error_bp): the relative error between the predicted results and the target output of the test set is calculated. The relative error indicates the degree of difference between the predicted value and the true value, which is defined as the difference between the predicted value and the true value divided by the true value.

b. Coefficient of Determination (R2_bp): measures how well the model fits the test set data. The coefficient of determination indicates the degree of correlation between the predicted values and the true values, and its value ranges from 0 to 1, with closer to 1 indicating a better fit.

4 Evaluating neural network models

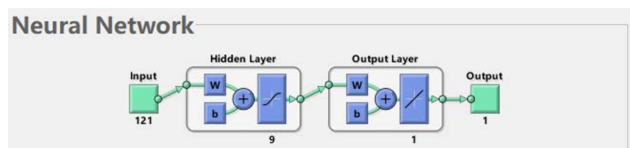

Figure 6 Neural network structure

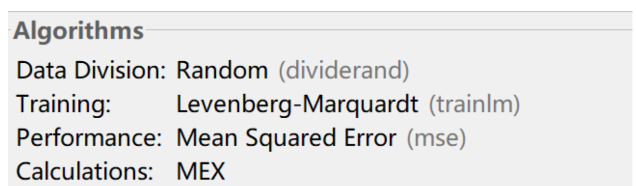

Figure 7 Neural network algorithm

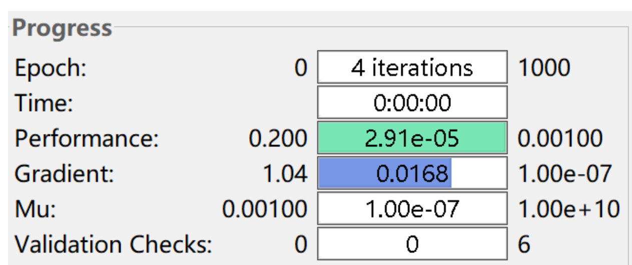

Figure 8 Neural network progress

From Figure 6 it is known that the size of the input layer of this neural network is 121 and the size of the hidden layer is 9. From Figure 7 it is known that the data division algorithm of this neural network is Random (dividerand), the training algorithm is Levenberg-Marquardt (trainlm) and the error algorithm is Mean Squared Error (mse). From Fig. 8 present study know that the number of iterations is 4, the error (performance) is 2.91e-05, the gradient (Gradient) is 0.0168 and the Mu value is 1.00e-07.

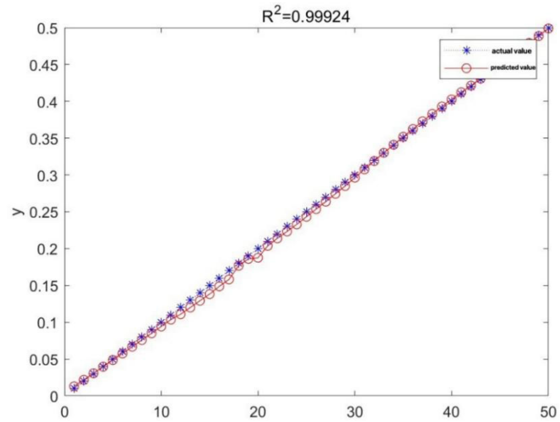

Figure 9 Comparative graphical representation

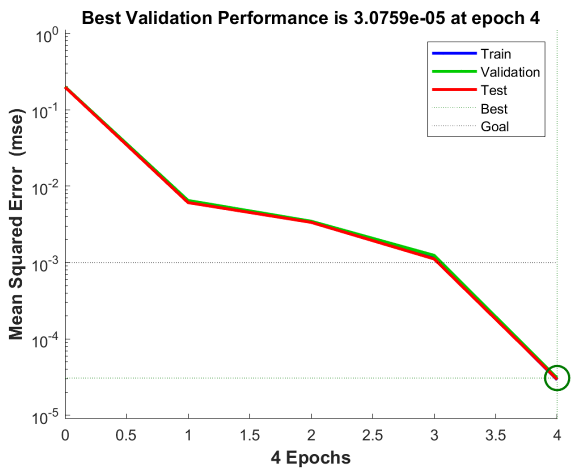

Figure 10 Error graphical representation

From the result Figure 9, it can be seen that the variance is only 0.99924, and the predicted values are well fitted to the true values.

Figure 10 shows the error plot (LOTS Performance): visualization of the error transformations during network training. best Validation Performance is 3.0759e-05.

Figure 11 shows the Training State: visualization of the gradient, Mu factor and generalization ability transformations during network training. gradient = 0.016751, Mu = 1e-07.

Figure 12 shows a graphical representation of the regression curves (Regression): a visualization of the regression power of the network training set, validation set, and test set.Training: R=0.99962, Validation: R=0.99963, Test: R=0.99961, All: R=0.99962, Output ~= 1*Target + -0.0063, Output ~= 1*Target + -0.0066.

To summarize, the number of iterations is 4. With only 4 iterations, the model has achieved a good performance. This indicates that the model was able to converge and find the appropriate parameter configuration with a relatively small number of iterations. The error (performance) is 2.91e-05, which is a small value indicating that the difference between the model's predicted and true values is small. This means that the model has high accuracy in predicting the optical performance of the point defect microcavity. The Gradient (Gradient) is 0.0168, and the smaller value of the gradient indicates that the adjustment of the model parameters is relatively smooth. This indicates that the training process of the model is relatively stable and there is no instability caused by too fast parameter tuning.The Mu value is 1.00e-07, and a smaller Mu value indicates that the model uses smaller steps for parameter updating during the training process. This setting helps to avoid too fast parameter adjustment and maintains the stability of training.

The best validation performance is 3.0759e-05 and the coefficient of determination (R) for the validation set is 0.99963: this indicates that the neural network model is able to accurately predict the optical properties of the point-defect microcavity of a two-dimensional GaAs dielectric-background photonic crystal during the training of the model and achieves excellent performance on the validation set. The small validation performance values and the coefficient of determination close to 1 indicate that the model has good generalization and fitting ability.

The coefficients of determination (R) for the training set, the test set and the overall dataset are all close to 0.99962-0.99963: this means that the model adapts well to the training data and produces highly correlated predictions on the test set and the overall dataset. This further supports the generalization ability and reliability of the model.

Linear relationship between output and target: Based on the equation for the linear relationship between output and target, it can be seen that there is an approximately linear relationship between the output of the model and the target. This linear relationship can be expressed by a simple linear equation where the output is approximately equal to the target multiplied by one minus a constant term (-0.0063 or -0.0066). This indicates that the model uses a linear approximation for predicting the optical properties of the point-defect microcavity.

Therefore approximate the expression:

Output ~= 1 * Target + (-0.0063)

Output ~= 1 * Target + (-0.0066)

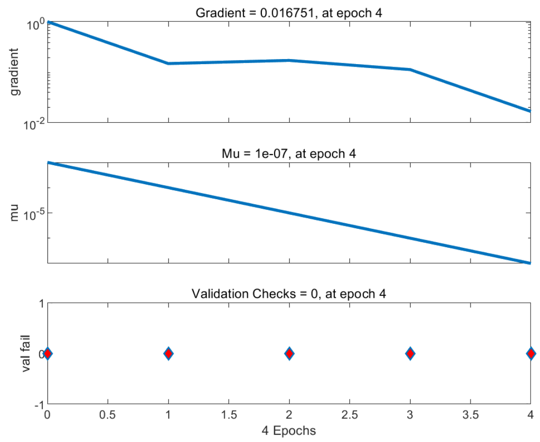

Figure 11 Graphical representation of the status of training

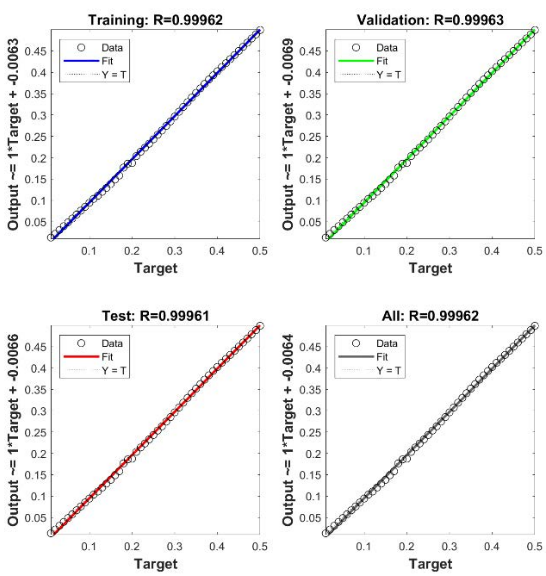

Figure 12 Graphical representation of the regression curve

These two equations represent the linear approximation used by the model for predicting the optical properties of point-defected microcavities in two-dimensional GaAs dielectric background photonic crystals.

Summary and outlook

The aim of this thesis is to establish a neural network model of point-defect microcavities in two-dimensional GaAs dielectric background photonic crystals and to use the model to predict and optimize their optical properties. By constructing a photonic crystal structure, introducing a point-defect microcavity and performing data acquisition, present study obtained sample data of the energy band structure of the photonic crystal. Then, present study designed and trained a BP neural network model using the energy band data of the photonic crystal as a training set for accurate prediction of the optical properties and optimization of the design, and finally succeeded in building a neural network model capable of quickly and accurately predicting the optical properties of the photonic crystal.

Through this study, the following results were achieved

(1) A neural network model for point-defect microcavities of two-dimensional GaAs dielectric background photonic crystals has been developed, which is capable of predicting the optical properties of photonic crystals quickly and accurately.

(2) Through the application of the model, present study are able to solve the challenges faced by traditional methods in designing and optimizing photonic crystals and improve the efficiency of design and optimization.

(3) Combining the properties of photonic crystals and neural networks provides new possibilities for high-speed and efficient optical calculations.

In terms of practical applications, the results of this study have the following implications:

(1) Crystal device design and optimization: photonic crystal point-defect microcavities have important potential applications in optical devices, such as fiber optic communications and lasers. With the established neural network model, present study are able to quickly and accurately predict and optimize the optical properties of photonic crystals, providing an efficient method for the design and optimization of novel crystal devices.

(2) Saving time and cost: Traditional methods require a lot of trial-and-error and optimization during the design and optimization of photonic crystals, which is time-consuming and not efficient enough. The neural network model can achieve nonlinear mapping and prediction by learning the patterns and features of data, which greatly saves the time and cost of design and optimization.

(3) Promote the development of photonics applications: photonics has a wide range of application prospects in the fields of information technology, communication, energy and biomedicine. By accurately predicting and optimizing the optical properties of photonic crystals, present study can promote the development of photonic devices and photonic integration technologies, and provide more efficient and reliable solutions for applications in these fields.

Conclusion

The results of this study provide a fast and accurate method for the prediction of optical properties and optimal design of point-defect microcavities in two-dimensional GaAs dielectric background photonic crystals. However, there are still some aspects that can be further extended and improved to make it more valuable for practical applications.

First, further experimental validation is necessary to verify the accuracy and feasibility of the neural network model. By comparing with the experimental data, the predictive ability of the model can be evaluated and the performance of the model can be further optimized. In addition, feedback from experimental data can be used to adjust the parameters and structure of the model to improve its accuracy of prediction and optimization.

Second, future research can consider introducing multi-scale and multi-parameter analysis to more comprehensively and accurately characterize the performance of photonic crystals. The performance of photonic crystals is often affected by several factors, such as the size of the structure and the nonlinear properties of the material. Therefore, combining neural network models with other modeling methods, such as finite element methods or optical simulation software, allows for the consideration of more complex optical effects and material properties.

In addition, the application of neural network models to real-world photonic device design and optimization can be further explored for its practical effects in engineering design and industrial applications. Close collaboration with engineers and industry will help customize the design and optimization to meet the needs of different application areas and accelerate the translation and commercial application of photonics technologies.

Finally, photonic crystal point-defect microcavities are often an integral part of photonic devices, and integrating them into systems with other optical components is critical for practical applications. Future research could apply neural network models to photonic device integration and system-level design, taking into account the interactions and optimization between different components to achieve more efficient and stable optical systems.

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