International Journal of Materials Science and Technology Studies

ISSN: 3006-7693 (Print), ISSN: 3006-3744 (Online) | Volume 1, Number 1, Year 2024
DOI: https://doi.org/10.62051/ijmsts.v1n1.13
Journal homepage: https://wepub.org/index.php/IJMSTS/index

Two-dimensional silicon-based dielectric column photonic crystal point defect microcavity Neural network modelling

Tingshuang Zhang

School of engineering, Yanbian University, Yanji, Jilin, 133002, China
1214022865@ybu.edu.cn

ABSTRACT

In order to solve the problem that it is difficult to predict the microcavity photonic energy bands of point defects in two-dimensional silicon-based dielectric column photonic crystals, this paper proposes a method to predict the microcavity photonic energy bands of point defects in two-dimensional silicon-based photonic crystals by using an artificial neural network model. In this paper, the energy band structure of triangular lattice point defects at different radii is calculated using MPB, and a neural network model is established based on this data and the accuracy of the established model is verified.

KEYWORDS

Photonic crystal; Silicon base; Point defect; Neural network modelling

1. INTRODUCTION

A photonic crystal is an artificial microcrystalline structure consisting of a periodic arrangement of materials with different dielectric constants, so named because the propagation of electromagnetic waves in it can be described by an energy band theory similar to that of the propagation of electrons in a semiconductor. Since John and Yabolonivitch proposed the concept of photonic crystals, research on photonic crystals has been carried out for more than 30 years, and photonic crystals have been widely and intensively studied by researchers due to their important research prospects in the fields of integrated optoelectronics, quantum optics, and so on [1, 2].

Silicon is a fundamental material for the modern integrated circuit industry and is one of the most mature materials in terms of preparation processes. Silicon has a high refractive index, which meets the requirements for generating a complete photonic band gap and special propagation effects of light, and it is transparent to the wavelengths used in the field of communications. Moreover, photonic crystal devices made from silicon are easy to be combined with conventional electronic devices, so silicon-based photonic crystals are a hot spot for research at present.

One important property of photonic crystal is to introduce defects in its periodic structure, which destroys its periodicity, and thus localised defects appear in the energy gap of the photonic crystal. Defective photonic crystals can be applied in waveguides, filters and other photonic crystal devices. Photonic crystal microcavity compared with the traditional resonant cavity, has a high quality factor, small device size, high detection accuracy and not subject to electromagnetic interference and other obvious advantages, and has become an international research hotspot. For example, if the transfer frequency between the ground state and the excited state of an atom falls within the bandgap region of a photonic crystal, the excited state of the atom cannot be coupled to any radiation mode. In this way, spontaneous radiation is strictly suppressed, resulting in the atom remaining in the excited state.

Localised defects in the vicinity of the atom have the opposite effect and can significantly increase the spontaneous emission rate.

Therefore, how to design photonic crystal point-defect microcavities has received a lot of research. Conventional design of photonic crystal devices requires the adjustment of geometrical parameters to try a large number of combinations in order to obtain the desired band structure. Moreover, designing using simulation methods requires a lot of time and is demanding on equipment such as computers.

In recent years, deep learning has grown rapidly and has been used in a wide range of fields. It is also heavily used in the study of optics and electromagnetism [3, 4]. Deep learning has been used in some studies to design optical devices and solve problems inversely. This method of designing optical devices usually requires a large number of iterative simulations, which is not intuitive and relies heavily on the experience of researchers. Artificial neural networks, on the other hand, can handle nonlinear and complex problems very well. A well-trained artificial neural network model requires less design time than traditional design methods. Artificial neural network models offer great possibilities to inverse design optical devices, i.e., artificial neural network models can design devices according to the user's needs. In this paper, bp neural network is used to update the weights and bias using back propagation algorithm, which can quickly adjust the network parameters to minimise the loss function, and compared to other neural network structures, BP neural network can learn complex mapping relationships more efficiently through back propagation. In addition, the training process of BP neural networks can be tuned by adjusting the network structure, choosing appropriate activation functions and optimisation algorithms to further improve the performance of the model. This flexibility allows BP neural networks to adapt to different types and sizes of datasets and achieve better generalisation capabilities.

What's more, the transfer function of BP neural network is generally a Sigmoid-type differentiable function, which can show a better balance between nonlinearity and linearity, and is a strictly increasing function, which can theoretically realise the nonlinear mapping between any inputs and outputs, and it is very suitable for prediction. Therefore, this paper adopts the method of establishing and training BP neural network to predict the microcavity radius of point defects in 2D Si-based dielectric column photonic crystals.

The aim of this paper is to train BP neural networks for predicting the radius of point-defect microcavities in two-dimensional silicon-based dielectric column photonic crystals. In the training process of the artificial neural network, the eigenfrequency is the input information and the radius of the point defect microcavity is the target. The dataset in the training process is obtained by the plane wave expansion method through the MPB programme.MPB (MTI Photonic-Bands package) is an open source crystal calculation software developed by Massachusetts Institute of Technology (MIT), which is very powerful, and this software is based on the plane wave expansion method, and can be used to efficiently calculate the energy-band structure of photonic crystals. Meanwhile, this paper compares the results of calculating by plane wave expansion method and the prediction by artificial neural network using the data which is not in the training set.

2. ACQUISITION OF EXPERIMENTAL DATA

This paper investigates the TE mode of a two-dimensional silicon-based dielectric column photonic crystal with point-defect microcavities. The photonic crystal consists of an air hole and a Si-based dielectric column. The basic parameters are: the background material is the air dielectric constant$\varepsilon_0 = 1$, the Si-based dielectric columns$\varepsilon_a = 12$, the point defects are the Si-based dielectric columns with different radii$\varepsilon_b = 12$, the base dielectric columns are arranged in a triangular structure in the air, and the point defect microcavities are the Si-based dielectric columns replaced by Si-based columns with different radii. The structure is shown in Figure 1.

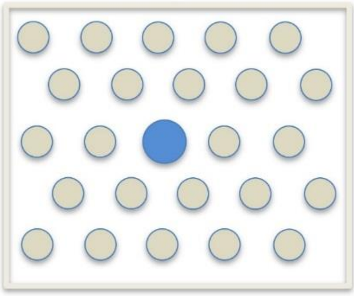

Figure 1. Schematic structure of point defect microcavity in 2D Si-based dielectric columns

Using the Massachusetts Institute of Technology's Photonic Banding (MBP) software package, 10 bands of 12 k-points were calculated for photonic crystals of 50 silicon columns with a background medium of air, a triangular lattice radius of 0.2, and a point-defected microcavity with a radius of 0.01 at intervals of 0.01 from 0.01 to 0.50 using the 16×16×16 grid-point discrete unit cell, respectively.

The data obtained from the calculation, after deleting the prompt line, to get a pure digital matrix containing k points of information wave vector size and band 611×15, imported into Matlab for data processing, which will be the same radius point defects of the frequency of the band in accordance with the fear of the number of bands in order to increase the number of k points in order to increase the order of the same line, and at the end of the line to add the corresponding radius, and in the direction of columns from the top to the bottom of the point defects radius Increased sequentially, the dataset was obtained and the dataset was saved.

In order to get a larger dataset so that the artificial neural network can be better trained and tested. The dataset is copied one hundred times in the row direction to generate a matrix at 5000×121, which is transposed to randomly select 4950 columns as the training set and the rest of the columns as the test set. The last row of the matrix is used as the output and the first 120 rows are used as the inputs for partitioning in the test set and the training set, respectively, the input of the training set is "P_train", the output of the training set is "T_train", the input of the test set is "P_test" and test set output "T_test". The obtained data set is shown in Figure 2. At this point, the data processing required for this paper is completed.

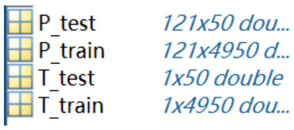

Figure 2. Processed data set

3. BUILD AND TRAIN ARTIFICIAL NEURAL NETWORKS

In this paper, we use Matlab's own functions to build an artificial neural network, and we need to determine the number of BP neural network layers before building the model, and it has been shown that an artificial neural network containing one hidden layer can approximate any continuous function [5], so a three-layer BP neural network can complete the required mapping. In this paper, an artificial neural network containing a three-layer structure is used as a basic model for predicting point-defective microcavities in silicon-based dielectric column photonic crystals. Combining the theory of fangfaGorman $S = log_2 N$,the number of hidden layer nodes of the network is set to 7 due to the input parameter of the network is 121 [6].The BP neural network is trained by using the Levenberg-Marquard algorithm to optimise the traditional neural network so as to obtain the better weights and thresholds. The artificial neural network was initially tested and trained at several different rates, and the errorsum of square was compared after training the neural network at different rates. if this value can be reduced quickly, it means that the chosen learning rate is more ideal. When the value decreases slowly or shows large oscillations, the current learning rate is not suitable. When the learning rate is too large, it will lead to a system that cannot be stabilised and unacceptable oscillations will occur, while a learning rate that is too small will lead to a situation where the convergence speed is too slow. The learning rate was finally set at 0.6 by comparing multiple this experiments.

Simulation experiments are carried out in Matlab with the following steps

(1) Create a neural network (functions from Matlab's Neural Network Toolbox, below)

net = newff (P_train,T_train,7);

(2) Setting training parameters

net. trainParam. epochs = 10000;

net. trainParam. goal = 1e-4;

net. trainParam. lr = 0.6;

The procedural statement indicates that the maximum number of training is 10000, the training accuracy is 1×10^{-4} , and the learning rate is 0.6.

(3) Training a neural network using a training set

net = trai, P_train, T_train).

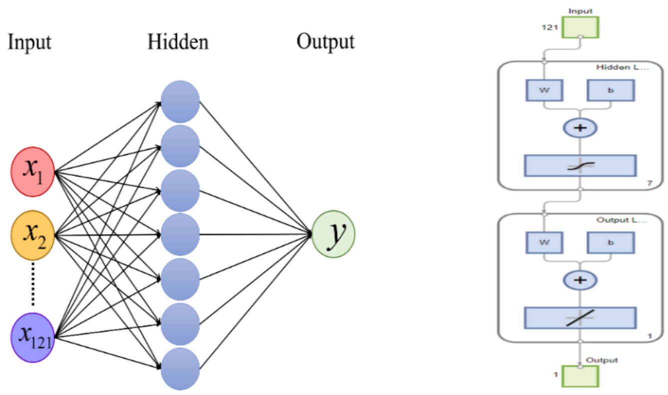

Figure 3. Neural Network Structure

4. TESTING NEURAL NETWORK PERFORMANCE

In this paper, the coefficient of determination R^2 is used in testing the accuracy of neural networks to assess the predictive power of the trained artificial neural network, i.e. how accurately the model is able to predict the output for the given data. R^2The value of ranges from 0 to 1. When R^2 is close to 1, it indicates that the model is able to explain the variability of the observed data well and the prediction is good, while when R^2 is close to 0, the model fails to explain the variability of the observed data effectively and the prediction is poor. R^2denotes the proportion of variance explained by the model, i.e., the proportion of actual observed data that can be explained by the model. Its calculation formula is:

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} \quad (1)$$

SS_{tot} is the total sum of squares:

$$\mathrm{SS}_{tot} = \sum_{i=1}^{n} (Y_i - \bar{Y})^2 \quad (2)$$

Where$\bar{Y}$ is the mean of the observations.

SS_{res} is the residual sum of squares:

$$SS_{res} = \sum_{i=1}^{n} (\hat{Y}_i - Y_i)^2 \quad (3)$$

Also, the output of the test set and the output predicted using the neural network and the coefficient of determination are plotted in a graph as shown in Figure IV.

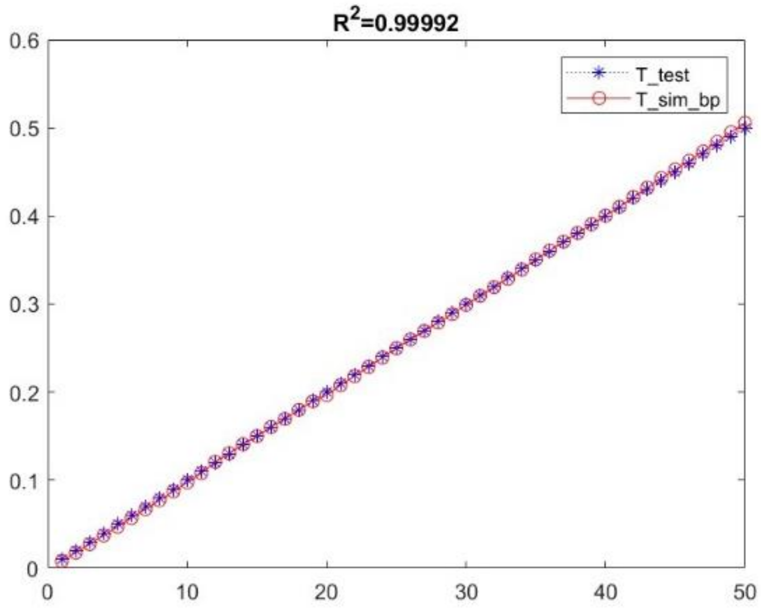

Figure 4. Analysis of measurement results

From Figure.4, it can be learnt that the coefficient of determination of the neural network model is 0.99992 which is very close to 1, and it can be intuitively seen from the image that the predicted value curve fits well with the real value curve. It shows that the trained artificial neural network can well explain the variability of the observed data, i.e., the radius of the point defect microcavity can be well predicted by the energy band structure of the photonic crystal point defect.

To analyze the neural network, in addition to using the calculated coefficients of determination of the decision, three plots of Training State, Regression, Performance in plots in the Matlab Neural Networks Toolbox were used, corresponding to Figures 5, 6, and 7, respectively.

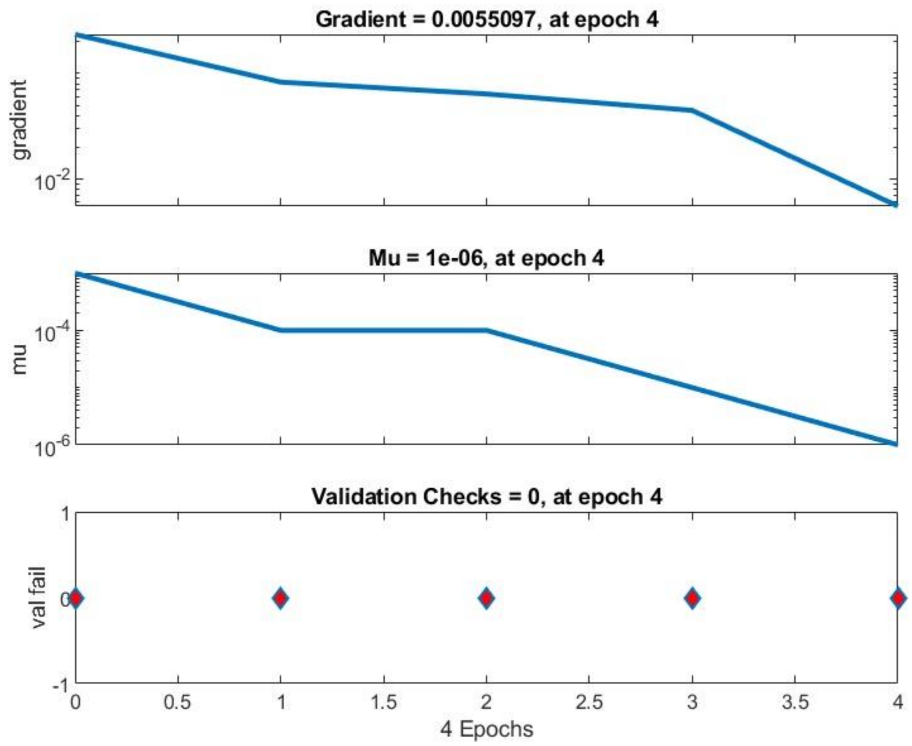

Figure 5. Training State

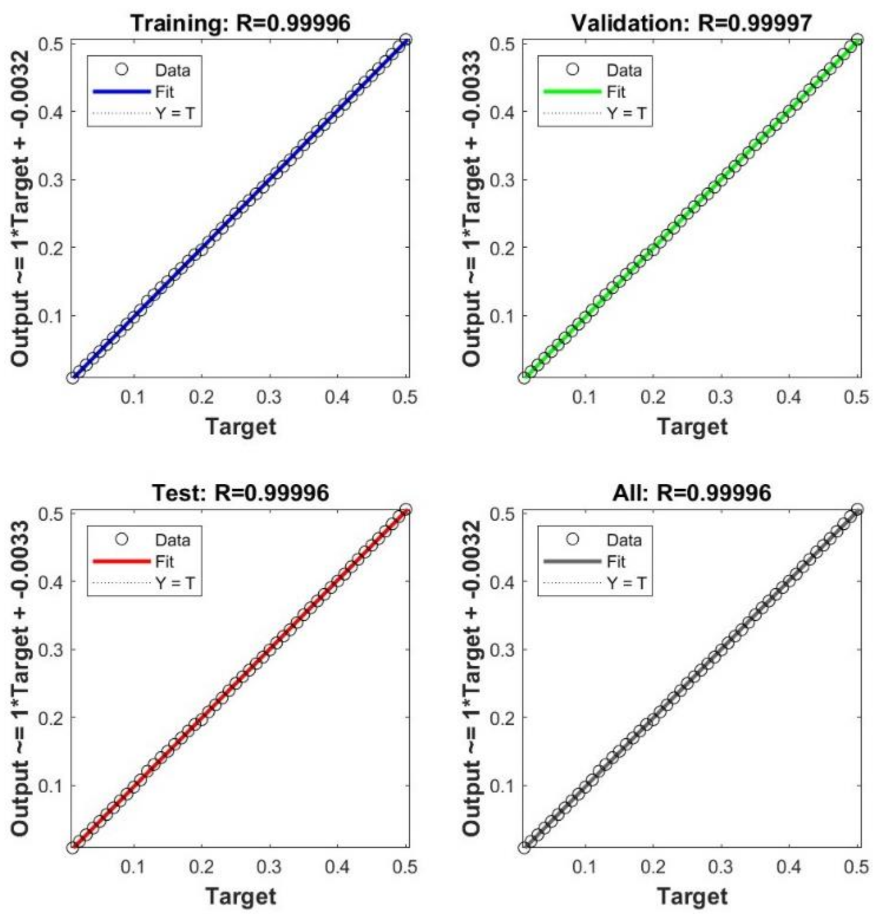

Figure 6. Regression

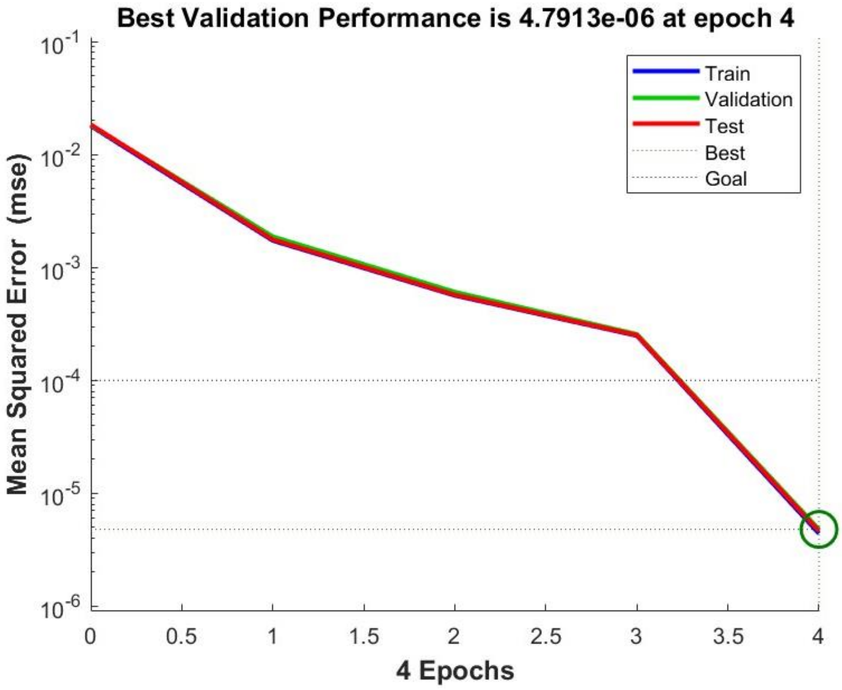

Figure 7. Performance

By Figure 5 Training State shows that only four rounds were needed to get the neural network model with the required accuracy indicating that the training speed was set reasonably well and the model could be trained quickly. Figures VI and VII both show that the data from training, validation, and testing in this model fit quite well. It also illustrates the accuracy and reliability of the model in this paper in predicting the microcavity radius of point defects in Si-based dielectric column photonic crystals.

5. CONCLUSION

In this paper, the band structure of two-dimensional triangular lattice silicon-based dielectric photonic dot defective microcavities is calculated. Where wave vectors, number of bands and corresponding frequency features are used to train the neural network model. The model is used to design 2D silicon-based dielectric column photonic crystal point defect microcavities. The results show that the trained artificial neural network model can predict the radius of the point defect microcavity well based on the desired photonic energy band structure.

REFERENCES

[1] Yablonovitch, E. (1994). Photonic Crystals. Journal of Modern Optics, 41:173-194.

[2] Qiu C, Wu X, Luo Z, et al. (2021). Simultaneous inverse design continuous and discrete parameters of nanophotonic structures via back-propagation inverse neural network. Optics Communications, 483: 126641.

[3] Pavan, V. D. R., Nikhil, V., Dey, K., Umamaheswara Sharma, B., & Roy, S. (2023). Analysing group indices and dispersion characteristics of engineered photonic crystal waveguides using artificial neural network. Journal of Optics.

[4] Asano T, Noda S. (2018). Optimization of photonic crystal nanocavities based on deep learning. Optics express, 26: 32704-32717.

[5] Hecht-Nielsen, R. (1992). Theory of the backpropagation neural network. In: International Joint Conference on Neural Networks. Washington, DC. pp. 593-611.

[6] Xu S, Chen L. (2008). A novel approach for determining the optimal number of hidden layer neurons for FNN's and its application in data mining. In: 5th International Conference on Information Technology and Applic. Queensland. pp. 683-686.