

Design of a Neural Network Model for Point-Defect Microcavities in Two-Dimensional Silicon-Based Dielectric Column Photonic Crystals

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Abstract: Currently, circuits are becoming more and more highly integrated, but current electronic chip technology has difficulty in meeting the requirements for increased data transmission speed and capacity because of its characteristics of increased energy loss due to interactions between electronic components. In contrast, photonic technology is a promising solution due to its characteristics of high speed, wide bandwidth, and low interaction. Photonic crystals are materials with an artificial periodic dielectric structure, with photonic bandgap and localization properties that are critical to their performance. Photonic crystals, which use photons as an information transfer medium, allow flexible control of photon propagation, just as electrons are controlled in semiconductors, and the study of multifunctional photonic crystals is important for the construction of integrated optical circuits. This paper proposes a neural network-based model to analyze and predict the optical properties of point defect microcavities in 2D silicon-based dielectric column photonic crystals. By modeling the complex relationship between the structural parameters of the photonic crystal and its optical response, a theoretical approach for the design of 2D silicon dielectric column photonic crystals can be provided.

Keywords: Photonic Crystal; Point Defect Microcavity; Neural Network Modeling.

1. Introduction

In the 1940s, researchers at Bell Laboratories in the U.S. developed the first transistor based on the semiconductor germanium, ushering in the era of electronics. Starting in the 1950s, people gradually entered the information age. With the emergence and development of several new information industries, such as online gaming, cloud computing, automated driving and the industrial Internet of Things, people not only put higher demands on data transmission speed, but also on data transmission capacity.

In 1987, Eli Yablonovitch and Sajeev John published their pioneering work on two-dimensional structured photonic crystals using silicon-based mesopillars and point defect microcavities. They also studied 2-D and 3-D photonic crystals and made important advances in the dispersion and confinement of light in these materials.

In 1996, Thomas Krauss developed the world's first optical quality 2D photonic crystals. This major technological breakthrough was the successful mass production of semiconductor-based photonic crystals using semiconductor fabrication techniques, which laid the technological foundation for a wide range of potential applications, including increased LED efficiency, development of laser cavities, and even faster computer processors.

Because of the advantages of high transmission speed and large transmission bandwidth, photons are gradually becoming more visible to people and belong to dimensionless structures that can expand or contract proportionally according to changes in the wavelength (or frequency) used. Ordinary photonic crystal structures have no special requirements for the environment in which they are used, can operate at room temperature, and are easy to combine or adapt with other structures. These advantages have led to photonic crystal structures being more widely studied and applied.

Many materials, structures and fabrication methods are currently used for photonic crystals. Among them, microfabrication techniques have advantages, such as not only high precision, but also saving materials and energy, facilitating multifunctional high integration and mass production. Then, two-dimensional structures can realize most of the characteristic requirements of photonic crystals, planar fabrication technology is mature and widely used, and the structure and use of one-dimensional photonic crystals is relatively simple, while three-dimensional photonic crystals have the disadvantages of structural problems with microfabrication and high cost. There are many materials that can be used in photonic crystals, but silicon has always been the most fundamental material, not only because of its high relative refractive index, but also because of its abundance of raw materials and advantages of stability and reliability in optoelectronic performance.

2. Significance of Research

Photonic crystals are special artificial structures composed of a periodic lattice of spaces with different dielectric refractive indices, which can be divided into three types according to the periodic lattice of dielectrics of this special nature: one-dimensional photonic crystal, two-dimensional photonic crystal and three-dimensional photonic crystal [1], as shown in Figure 1.

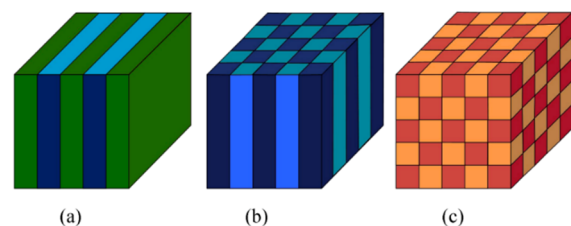


Figure 1. Types of photonic crystals

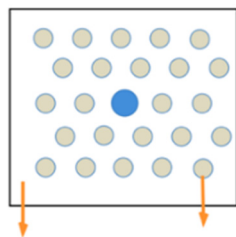
By introducing point defects into photonic crystals, it is possible to design photonic crystal microcavities with smaller mode volumes and higher quality factors than ordinary silicon resonant cavities. Two-dimensional silicon-based photonic crystals have a dielectric column structure and an air hole structure. By removing, moving, changing or adding air holes in two-dimensional planar air-hole photonic crystal structures and disrupting the periodic structure of the photonic crystal, it is possible to construct point-defect microcavities in the photonic crystal[2]. Currently, H0 cavities, H1 cavities, L3 cavities, Ln cavities and ring cavities[3] are the focus of research on point-defect microcavities in photonic crystals.

Silicon is one of the basic materials for the preparation of photonic crystals, especially two-dimensional silicon-based photonic crystals, which can meet most of the characteristic requirements of photonic crystals and have the advantages of easy processing, high structural precision, easy integration and mass production. The application of two-dimensional silicon-based photonic crystals has expanded from the fields of mirrors, lasers, waveguides, fiber optics and solar energy to multiple fields, such as terahertz devices, big data transmission, photonic chips, bio-detection and stealth technology [4].

In this paper, author provides a theoretical method for the design of two-dimensional silicon-based dielectric column photonic crystals by establishing a point-defect microcavity neural network model in two-dimensional silicon-based dielectric column photonic crystals. Compared with traditional computational electrodynamic simulation, the deep neural network can significantly improve the speed of simulation and prediction while ensuring accuracy due to its higher adaptive expression capability. Through learning and training the relationship between inputs and outputs, this paper proposes to establish a deep learning-based model of point-defect microcavities in two-dimensional silicon-based photonic crystals to quickly and accurately predict the optical performance of point-defect microcavities, provide a theoretical basis for optimizing design and application, promote the development of photonic devices and photonic integration technology, and facilitate the application of photonics in communications and medicine.

3. Methods

3.1. Modeling of 2D Photonic Crystal Dielectric Columnar Dielectric Microcavities with Point Defects based on Silicon



Silicon-based material Air hole

Figure 2. Photonic crystals in silicon-based media

In this work, silicon (Si) with refractive index $n = 3.5$ was used for its excellent optical properties. A cylindrical dielectric column was introduced to form microcavities with point defects in the lattice as shown in Figure 2. The dielectric

column was composed of air with a pore refractive index $n = 1.0$, and the radius r was used as a tuning parameter. The specific effect of different microcavity sizes on the photonic crystal performance was studied by adjusting the radius in ascending order from 0.01 to 0.51 in increments of 0.01.

3.2. Data Collection

The project uses the MIT open-source model and Ubuntu virtual machine to carry out the study, using MPB to calculate the sample data of photonic energy bands, including different photonic crystal microcavity structures with point defects and the corresponding photon mode and scattering relations. Energy band calculations allow us to clearly observe the subtle changes in the photonic crystal energy band structure as the radius of the point defect changes.

In this paper, author take a systematic approach to analyze the energy band structure of photonic crystals in the context of a two-dimensional silicon (Si)-based medium in a study that explores the microcavity patterns of point defects in photonic crystals. First, author defines the key simulation parameters, such as the resolution and the number of energy bands, which are essential to ensure the accuracy of the computational results. Then author determines the positions of the points Γ and K' and generate ten K points between these two points as shown in Figure 3.

```
(set! geometry-lattice (make lattice (size 5 5 no-size)
  (basis1 (/ (sqrt 3) 2) 0.5)
  (basis2 (/ (sqrt 3) 2) -0.5)
))
(set! geometry (list (make cylinder
  (center 0 0 0) (radius 0.2) (height infinity)
  (material (make dielectric (epsilon 12))))))
(set! geometry (geometric-objects-lattice-duplicates geometry))
(map (lambda (r)
  (set! geometry (append geometry
    (list (make cylinder (center 0 0 0)
      (radius r) (height infinity)
      (material (make dielectric (epsilon 12)))))))
  (arithmetic-sequence 0.01 0.51 0.01)))
(set! resolution 16)
(set! num-bands 10)
(define Gamma (vector3 0 0 0))
(define K' (lattice->reciprocal (vector3 0.5 0 0))) ; edge of Brillouin zone.
(define K (vector3 0.5 0 0)) ; edge of Brillouin zone.
(set! k-points (interpolate 10 (list Gamma K')))
(run-te)
(print "r:" r "\n")
)
```

Figure 3. Calculated photon energy bands of point-defected microcavities of 2D Si-based dielectric column photonic crystals

To study in detail the influence of microcavities at point defects on the energy band structure of photonic crystals, author uses a cyclic iterative approach. In each iteration, cylindrical defects of different radii are added to the list of shapes and the value of the current radius is recorded as shown in Figure 4. In this way, a sequence of radii ranging from 0.01 to 0.51 is gradually constructed. This sequence not only shows the effect of defects of different sizes on the performance of the photonic crystal, but also provides a set of detailed samples to analyze the scattering relationships.

By fixing simulation parameters and adding cylindrical defects with different radii, author was able to construct a point defect microcavity model of a photonic crystal and study its energy band structure in detail. This approach not only provides a wealth of data for analyzing the effects of defects of different sizes on the performance of photonic crystals, but also demonstrates the potential application of systematic research methods in the field of photonics.

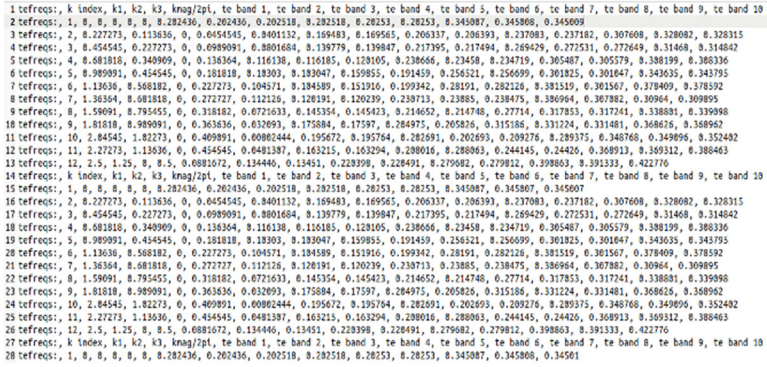


Figure 4. Photon energy bands in two-dimensional silica-based dielectric photonic crystals with point-defect microcavities at different radii

3.3. Designing the Neural Network Model

To build a reliable machine learning model, as shown in Figure 5, both data preparation and data processing are important, especially in the context of predicting the energy band structure of photonic crystals. First, an initial sample of photonic crystal energy band data was collected. These data typically include the optical properties of different photonic crystal structures with different parameters. Second, a data augmentation strategy was applied. In other words, the data set was artificially enlarged by copying and slightly modifying the original data sample. This not only increases the diversity of the data, but also improves the generalizability when training the model[5].

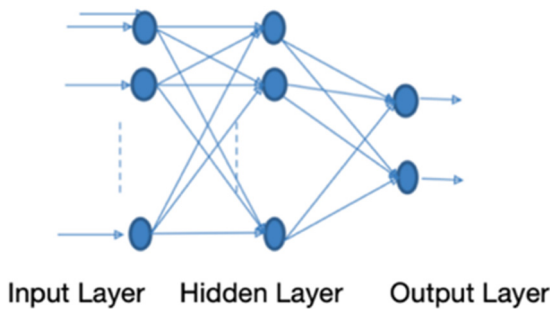


Figure 5. Machine learning model

The extended data set is then divided into two parts, a training data set and a test data set, so that the model can be effectively validated using independent data. Typically, the training dataset is used to train the model and fit the parameters, while the test dataset is used to evaluate the model performance with unknown data.

In addition, techniques such as cross-validation are introduced to further improve the robustness and predictive accuracy of the model. By dividing the dataset into several groups and repeating the training and testing on these groups, the model performance can be evaluated from multiple perspectives, leading to more comprehensive and reliable evaluation results.

During the creation of the BP neural network model, the BP neural network was selected as the model structure based on the characteristics of the dataset, and the neural network instance was initialized. During network creation, the complexity of the model was balanced with processing power by adjusting the size of the hidden layers, and in particular, the number of nodes in the input and output layers was

determined according to the number of features and target variables in the dataset, thus implementing an appropriate network structure.

3.4. Training the Neural Network Model

It then defines essential training parameters, such as training speed, number of iterations and target error limits, which control the training process, adjust model weights and ensure training efficiency. The training data is then used continuously to adjust the weights and mesh bias to minimize the difference between the predicted model outputs and the actual target values until the model reaches a predefined performance criterion. Once the model is trained, simulation tests validate its predictive ability. The test set is introduced into the trained network to obtain the model's prediction results for the new data. This step is not only important to evaluate the performance of the model, but also provides an intuitive indication of its generality.

Overall, author has successfully created a BP neural network model with excellent predictive ability for the properties of photonic crystals.

3.5. Evaluating Neural Network Models

In conducting a comprehensive performance evaluation of the machine learning model, two key metrics were used to analyze in detail the accuracy and goodness of fit of the model. First, the relative error, an intuitive measure of the model's predictive accuracy, was obtained by calculating the proportional difference between the predicted and actually observed values of the model. When evaluating the performance of a model, a small value of the relative error means that the model is able to make accurate predictions with low bias.

In addition, the coefficient of determination, also known as the R-square value, is entered to measure the degree of agreement between the model's predicted values and actual values. A high value of the coefficient of determination indicates a high degree of agreement between the model and the data, indicating that the model is able to capture the underlying pattern of the data; an R-square value close to 1 generally means that the model has a very good fit and can reliably predict unknown data. Figure 6 shows that the coefficient of determination is only 0.94266, indicating a high degree of agreement between predictions and actual observations.

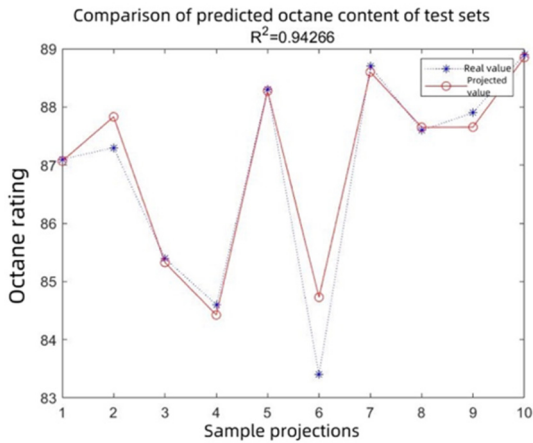


Figure 6. Comparison

Figure 7 shows that the model performs well after only three iterations, with a best validation performance of 0.35226. Analyzing the microcavity optical performance prediction models for point defects, there are several important performance indicators that indicate high model efficiency and stability. The low error values indicate very small deviations between the model-predicted results and the actual situation, reflecting the high efficiency of the model in accurately predicting the optical performance of the target.

Figure 8 provides an intuitive visualization of the main dynamic changes that occur during network learning, such as changes in the gradient, adjustment of the mu coefficient and changes in the generalizability of the model. The figure shows that the value of the gradient remains at 0.30516 during the learning process. This low value of the gradient indicates that the adjustment of the network weights is smooth. At the same time, the mu coefficient is fixed at a very low value of 1e-06, which also indicates that the neural network ensures the stability of learning and reduces the risk of overfitting.

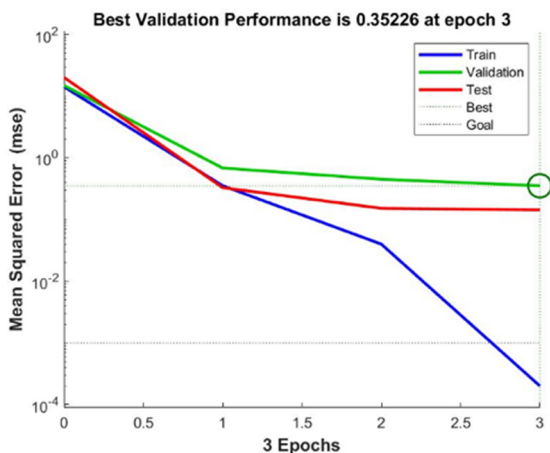


Figure 7. Inaccuracy

Figure 9 shows the results of the regression analysis of the network on the training, validation and test datasets. The regression curves in this figure show the performance of the network on the different data sets: on the training set, the R value is close to 0.99995, indicating a very high fit. For the validation set, the value decreases slightly to 0.93378, but still reflects the high accuracy of the model. Overall, the R value for all data combined is 0.98249, and all R values are stable in the range between R = 0.93378 and R = 0.99995, indicating

that the model has a very good overall fit. These data reflect the high accuracy of the model for the specific dataset and reveal the excellent complexity of the model and its generality.

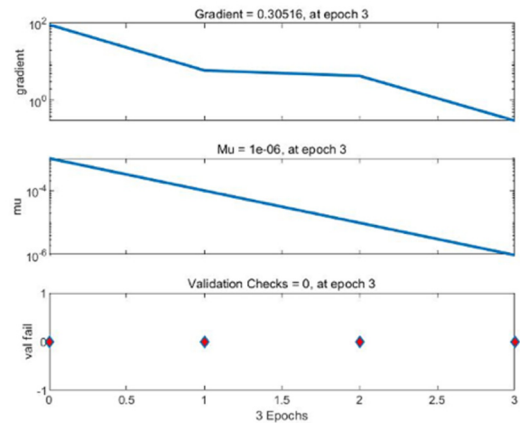


Figure 8. Training set

Overall, this study demonstrates a model that converges rapidly and achieves high prediction accuracy with a small number of iterations. Through careful tuning of parameters and learning strategies, the model not only maintains efficient prediction performance but also ensures stability during the learning process. These features enable the model to predict well the optical performance of microcavities with point defects, providing a valuable reference for research in related fields.

4. Conclusion

This paper describes the construction of a neural network model of a photonic crystal with point defects in a 2D silicon-based medium, used to analyze and predict the optical properties. A BP neural network model was then constructed from the collected data samples and used as a learning base to improve the prediction accuracy of the photonic crystal's optical properties through model learning. The research results show that the developed neural network model can quickly and accurately predict the optical performance of photonic crystals. Moreover, the success of this study not only highlights the potential of using advanced machine learning techniques to solve traditional physics problems, but also provides a new methodology for photonic crystal design and performance optimization. Author believes that the application of this model will play an important role in improving the efficiency of photonic crystal design, reducing costs and developing photonic applications.

Through this work, it is now possible to predict the great potential of neural networks in predicting the optical properties of point-defect microcavities in photonic crystals. The model's high accuracy, excellent generalizability, and clear and unambiguous linear relationship between predicted results and actual values demonstrate that neural networks can be used for such complex prediction tasks. In the future, these results will provide valuable insights for the design and optimization of photonic crystals and facilitate the development of related fields.

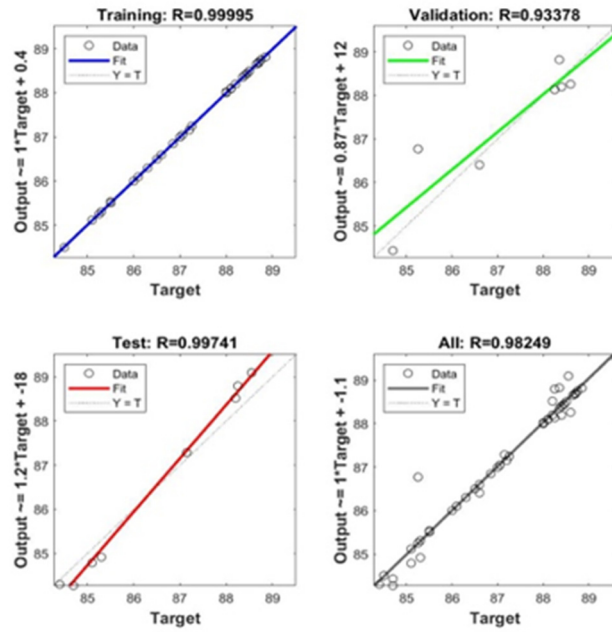


Figure 9. Regression curve

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