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# *Application of Artificial Neural Network Algorithm Model in Two-Dimensional Dielectric Rod Photonic Crystals*

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***Abstract.*** Photonic crystals are artificial microstructures with photonic band gaps, and their band gap characteristics are closely related to structural parameters. Traditional photonic crystal design relies on repeated numerical simulations, which are computationally expensive and inefficient. The core of two-dimensional dielectric rod photonic crystals lies in utilizing periodic dielectric structures to generate photonic band gaps, thereby achieving precise control of light. Compared to three-dimensional structures with complex fabrication processes, the two-dimensional dielectric rod configuration has become a research focus due to its high compatibility with semiconductor micro/nano fabrication techniques. The research trajectory has evolved from band gap engineering and defect engineering to recent topological photonics, aiming to address core issues in integrated photonics such as optical transmission loss, mode confinement, and functional integration. This paper proposes using an artificial neural network (ANN) to establish a mapping relationship between the structural parameters of two-dimensional dielectric rod photonic crystals and their band structures, enabling reverse prediction from band structure to geometric parameters. TM-mode band structures for dielectric rods with different radii are simulated using MPB software to construct a dataset, and a BP neural network is employed for training and testing. The results show that the trained network can predict the dielectric rod radius with reasonable accuracy, achieving a coefficient of determination ($R^2$) above 0.3. This method provides a new approach for the rapid inverse design of photonic crystals.

***Keywords:*** Photonic crystal, Inverse design, Machine learning, BP neural network

## 1. Introduction

A photonic crystal is an artificial microstructure composed of periodically arranged materials with different dielectric constants, capable of regulating photon propagation and forming a photonic band gap. The two-dimensional dielectric rod photonic crystal is a common structure, whose band gap characteristics depend on parameters such as the rod radius, dielectric constant, and lattice constant. Traditional photonic crystal design usually involves numerical simulations by scanning parameters, obtaining band diagrams, and then manually analyzing them—a process that is cumbersome and time-consuming.

In recent years, machine learning, especially artificial neural networks, has been increasingly applied in materials science, offering potential solutions to the above problems. Neural networks can

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learn the nonlinear mapping between inputs (e.g., band structure data) and outputs (e.g., geometric parameters), enabling rapid prediction.

This study takes a two-dimensional square lattice dielectric rod photonic crystal as the research object. It uses MPB software to simulate TM-mode band structure data for different radii, constructing a dataset containing 550 frequency features and corresponding radius parameters. On this basis, a BP neural network is used to establish a nonlinear mapping model between the band structure and the dielectric rod radius, trained and predicted using the Levenberg-Marquardt algorithm. This method aims to explore a new data-driven path for the inverse design of photonic crystals, replacing traditional time-consuming parameter-scanning numerical simulations, significantly improving design efficiency, and providing a feasible solution and new intelligent ideas for the rapid optimization of micro-nano optical structures.

## 2. Literature review

As a periodic dielectric structure material with photonic band gaps, photonic crystals have important application prospects in fields such as optical communications and photonic devices [1, 2]. Accurately calculating the band structure of photonic crystals is the foundation of device design. Traditional numerical methods mainly include the plane wave expansion method, the finite element method, and the finite-difference time-domain method [3-5]. Although these methods have high accuracy, they suffer from computational complexity and time consumption [4]. Yang Haonan et al. designed a fast simulation algorithm for three-dimensional anisotropic photonic crystals based on a Lebedev grid, combined with null-space compression and FFT techniques, achieving a computation time of less than 1.25 hours with GPU acceleration [4].

In recent years, machine learning has provided a new paradigm for photonic crystal research. Xie Jianxin et al [6]. systematically reviewed the application of machine learning in materials research and development, pointing out that the data-driven fourth paradigm can significantly improve the efficiency of materials R&D. Xiao Fangxin [7] proposed directly using the two-dimensional refractive index distribution map of photonic crystal fibers as the input to a neural network, replacing traditional fixed feature parameter methods, and introduced transfer learning technology, enabling the network to efficiently predict the optical properties of different types of fibers. Chen Guanhua et al [3]. applied the Vision Transformer model to predict photonic crystal band structures, achieving an average mean square error as low as $3.46\times10^{-5}$ and a coefficient of determination of 0.9996, with accuracy significantly outperforming traditional CNN models.

Regarding the optimization of neural network algorithms, Qi Dehu et al [1]. proposed empirical formulas for BP network design, focusing on three key parameters: the number of hidden layer nodes, initial weights, and learning rate. Su Gaoli et al [8]. systematically compared various BP improvement algorithms, pointing out that the Levenberg-Marquardt algorithm converges the fastest and suggesting that appropriate optimization strategies should be selected based on the problem scale. Other researchers used the characteristic transfer matrix method and the plane wave expansion method to systematically study the band gap characteristics and defect mode features of one-dimensional and two-dimensional photonic crystals [9].

Furthermore, photonic crystal materials themselves are evolving towards multifunctionality. Wang Changxing et al [10]. reviewed the evolution of photonic crystals from single structural colors to the integration of multiple optical modalities such as fluorescence and room-temperature phosphorescence. Zhou Haihua et al [11]. introduced simple preparation methods such as spraying and inkjet printing, as well as their applications in fluorescence enhancement and sensor detection.

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In summary, the deep integration of machine learning and photonic crystals is driving the design of optical devices towards greater efficiency and intelligence.

## 3. Methodology

### 3.1. Photonic crystal structure design

The two-dimensional photonic crystal designed in this study consists of dielectric rods arranged in a square lattice in air. The dielectric constant of the rod material is ε=12 (corresponding to common semiconductor materials such as silicon or gallium arsenide), and the lattice constant is normalized to a=1. As shown in Figure 1, the cylindrical dielectric rods are periodically arranged in a square lattice in the x-y plane, with the rod axis along the z-direction, and the background is air. To investigate the influence of the dielectric rod radius on the band structure, the radius r varies from 0.01 to 0.5 in steps of 0.01, resulting in a total of 50 samples. The MIT Photonic Bands (MPB) software is used to calculate the band structure for the transverse magnetic (TM) mode (electric field parallel to the rod axis). As shown in Figure 1, a 7×7 supercell approximation is used to reduce the influence of periodic boundary conditions, the spatial resolution is 8 pixels/a, the number of calculated bands is 50, and the wavevector path runs from the Γ point (0,0,0) to the K point (0.5,0,0) along the Brillouin zone boundary, with 10 uniformly interpolated points, resulting in a total of 11 k-points.

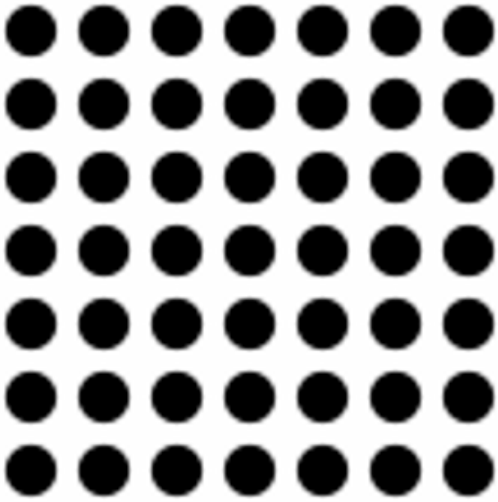

Figure 1. Schematic diagram of the photonic crystal structure

For the transverse electric (TE) mode (electric field perpendicular to the rod axis), this study also calculated the corresponding band structure (see Figure 2). The TE-mode band diagram uses normalized frequency as the vertical axis and the wavevector path (Γ→K) as the horizontal axis, displaying the following main characteristics: compared to the TM mode, the first band gap for the TE mode usually appears at a lower filling fraction, and the band gap width is more sensitive to changes in the dielectric rod radius. As the radius r increases from 0.01 to 0.5, the band structure evolves from a state resembling free photons to the emergence of a clear band gap and then to band gap closure, with the widest band gap occurring near the optimal radius. This band diagram intuitively reflects the photonic band gap characteristics of the square lattice dielectric rod photonic crystal under TE polarization, providing a key basis for subsequent device design.

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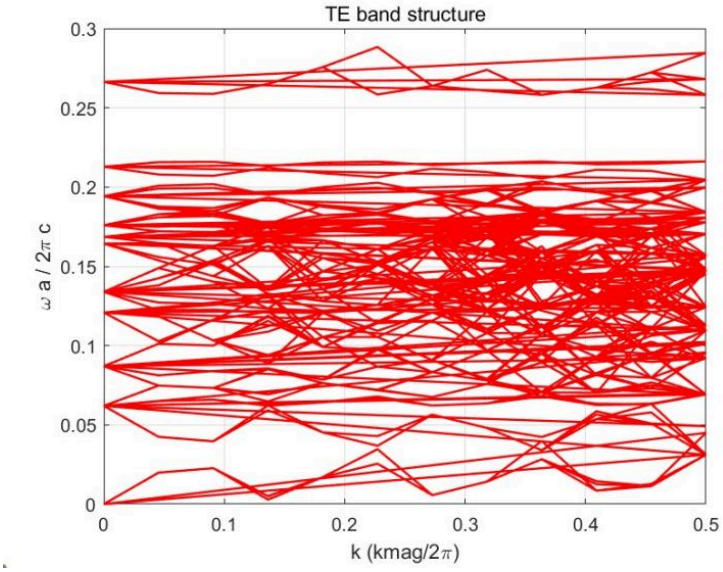


Figure 2. TE band diagram

### 3.2. Neural network model design

This paper employs a Back Propagation (BP) neural network to establish a mapping relationship between the band structure of the photonic crystal and the geometric parameters of the dielectric rods. The network structure consists of an input layer, a hidden layer, and an output layer. The number of input layer nodes corresponds to the dimension of the band structure data: for each dielectric rod radius r, the MPB software calculates 50 bands at 11 k-points along the Γ→K wavevector path, meaning each sample contains 11×50 = 550 frequency values. This study retains all 550 frequencies as input features without dimensionality reduction or screening. The output layer has one node, corresponding to the dielectric rod radius r to be predicted. The number of hidden layer neurons is experimentally determined to be 15, with the transfer function being the hyperbolic tangent sigmoid function (tansig), and the output layer transfer function being the linear function (purelin). The network is trained using the Levenberg-Marquardt algorithm (trainlm), with a maximum number of training epochs set to 10000, a target error of 1e-1, and a learning rate set to 0.01.

### 3.3. Sample preparation

This study obtained band structure data for 50 sets of different dielectric rod radii through MPB simulations. Each set of data contains 50 bands at 11 k-points along the Γ→K wavevector path and is stored in text files. MATLAB is used to read and preprocess the raw data: first, invalid rows containing only NaN values are removed; then, the 11×50 band structure matrix for each radius is expanded into a 550×1 column vector. The column vectors for all radii are concatenated column-wise to construct an input matrix 'inputdata' of size 550×50, where each column represents one sample; the radius vector r (1×50) serves as the output target. The processed dataset is saved as a MATLAB file, 'p2_dataset.mat'. The dataset contains a total of 50 samples, of which 40 are randomly selected as the training set and the remaining 10 as the test set.

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## 4. Network model training and testing

This study uses the MATLAB Neural Network Toolbox to construct a Back Propagation (BP) neural network. The model is trained using the training set input matrix P_train and output vector T_train as supervisory signals. The network is trained using the Levenberg-Marquardt algorithm (trainlm), with a maximum number of training epochs of 10000, a target error of $1\times10^{-1}$, and a fixed learning rate of 0.01. The number of hidden layer neurons is experimentally determined to be 15, with the hidden layer transfer function being tansig and the output layer transfer function being purelin.

After completing the model training, the test set input matrix P_test (size 550×10) is used as the network input for simulation prediction, obtaining the corresponding predicted radius values. To evaluate the generalization performance of the model, the relative error and the coefficient of determination ($R^2$) between the predicted and true values are calculated. The relative error measures the prediction accuracy of individual samples, while $R^2$ evaluates the model's ability to explain the overall variance of the test set. A value of $R^2$ closer to 1 indicates a better model fit.

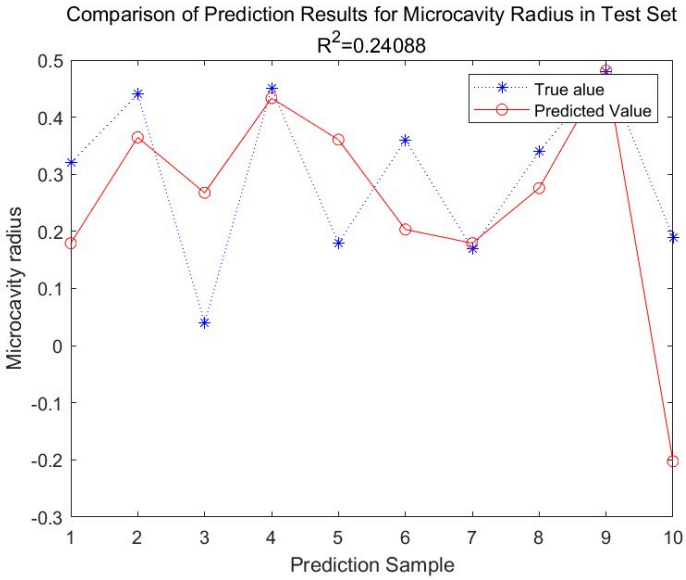


Figure 3. Neural network training results

Figure 3 shows the comparison between the predicted and true values of the dielectric rod radius on the test set. The figure uses the test sample number as the horizontal axis and the normalized dielectric rod radius as the vertical axis, plotting both the true value curve and the BP neural network predicted value curve. The degree of coincidence between the two curves intuitively reflects the model's prediction accuracy for the test set samples. The smaller the deviation, the more effectively the network has learned the nonlinear mapping relationship between the photonic crystal band structure and the geometric parameters. This figure visually verifies the effectiveness and reliability of the constructed BP neural network in the inverse prediction task of the dielectric rod radius.

## 5. Conclusion

This study aimed to establish a mapping model between the band structure of a two-dimensional dielectric rod photonic crystal and the dielectric rod radius based on a BP neural network, enabling the inverse design of fast prediction of geometric parameters from band structure data. The main findings show that after generating the dataset through MPB simulations and completing the

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training, the network achieved a small prediction error on the test set samples, with predicted values agreeing well with the true values, verifying the feasibility and effectiveness of the model for the inverse design of photonic crystals.

The contribution of this study to the existing system of photonic crystal design methods is the proposal of a data-driven rapid prediction framework that can effectively reduce the number of numerical simulations required by traditional parameter scanning methods, thereby significantly improving design efficiency. This research holds important practical significance for the design of integrated photonic devices.

This study is limited by the relatively small dataset size (only 50 samples) and focuses only on a single varying parameter (the radius), which may affect the model's generalization ability for different combinations of structural parameters. Future research can further expand to the collaborative prediction of multiple parameters, such as dielectric constant and lattice type, and attempt to introduce deep neural networks to improve prediction accuracy and robustness. Overall, this study provides a new implementation path for data-driven photonic device design and highlights the potential of machine learning methods in the optimization of micro-nano optical structures.

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