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Research Article

Performance Enhancement of Metasurface Grating Polarizer Using Deep Learning for Quantum Key Distribution Systems

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Abstract: Metasurface polarizers are essential optical components in modern integrated optics and play a vital role in many optical applications including Quantum Key Distribution systems in quantum cryptography. However, inverse design of metasurface polarizers with high efficiency depends on the proper prediction of structural dimensions based on required optical response. Deep learning neural networks can efficiently help in the inverse design process, minimizing both time and simulation resources requirements, while better results can be achieved compared to traditional optimization methods. Hereby, utilizing the COMSOL Multiphysics Surrogate model and deep neural networks to design a metasurface grating structure with high extinction ration of ≈60000 at visible spectral wavelength of 632 nm, could be achieved.

Keywords: metasurface, polarizer, grating, deep learning, neural network and surrogate model.

1. Introduction

Quantum cryptography is an innovative subfield of cryptography that leverages the principles of quantum mechanics in communication to provide distribute encryption keys. Different from classical cryptography, quantum cryptography is based on fundamental physics laws and is therefore highly immune to attacks by the most advanced computing systems. Quantum key distribution (QKD) is a secure communication protocol which utilizes quantum mechanics principles to distribute encryption keys [1]. Polarization encoding is the most used degrees of freedom to encode data in QKD system [2]. Polarizers are considered as essential optical components used in both transmitters and receivers of the QKD systems [3].

Metasurfaces, which are optical devices comprising structures on the nanometer scale and designed to control the wavefront and properties of light, are promising artificial materials to replace conventional optical components such as refractive optical elements (ROEs). Metasurfaces have the ability to manipulate various optical properties, including polarization, amplitude, and phase, within a single component. Besides, they provide the capability to reduce the form factor of bulky systems by replacing conventional optical elements [4].

The design of microscopic structures remains a major topic in metasurface optics research. Even though optical structure performance is typically straightforward to predict, through sophisticated simulation algorithms such as finite element method (FEM) and finite different time domain (FDTD), the problem of inverse designing an on-demand optical metasurface device is not that simple. At the early research, the prototypical designs were mostly based on educable guesses such as the split ring, V-shaped antenna, and gammadions. However, limited by the prior knowledge of humans and the sophisticated light-matter interaction mechanisms, exceptional functionalities and extremely high efficiencies may have never been discovered by intuitively guessed geometries. In order to overcome the difficulty of metasurface and optical design, inverse design methodologies, such as adjoint methods and evolutionary algorithms, have become one of the main themes of research in recent years. These algorithms have successfully been implemented for the design of different unconventional optical devices, such as power splitters, light trapping structures, and dielectric nano antennas. To further develop the capabilities of machine-aided design approaches, and to avoid some problems of traditional optimization, such as the local minimum problem and expensive computations, the optical community started to look at data-driven and machine learning methods as alternative approaches to resolve the inverse design problem. Hence, machine learning became the central research theme in computer vision, natural language processing, speech recognition, and more. The optical community has been increasingly migrating the techniques of machine learning and data science into optical research, with various successful applications including ultrafast optics, optical communication, and optical microscopy [5] [6].

Artificial intelligence (AI) recently became a global concept in various physical sciences. Specifically, there are a diversity of challenging tasks in optics that can be effectively analyzed and solved without directly solving Maxwell’s equations but by utilizing these novel approaches. Meanwhile, the direct solution of Maxwell's equations can be utilized to generate enormous amounts of training data required for executing various AI algorithms. Thus, a remarkably powerful AI methodology which complements many typical analytical and numeric techniques finds many key applications in optics. Such approaches are used for inverse design, optimization, big-data processing, underpinning the fast development of optics. The concept of all-dielectric metasurface is motivated by the idea to utilize subwavelength dielectric Mie resonant nanoparticles as “meta-atoms” to build high efficient optical metasurfaces and meta devices [7]. Those can be defined as optical devices having exclusive functionalities because of a smart structuring the meta-atoms at the subwavelength scale merged with the use of functional and high-refractive-index materials. Differs from classical optics, where the electromagnetic response is totally defined by electric polarization, the metasurface is frequently termed “meta-optics” highlighting the importance of optically induced magnetic response of the artificial subwavelength-patterned structures. The high-refractive-index materials provide exceptional confinement of electromagnetic fields making even subwavelength particles resonant. The interference between these resonances results in a sort of scattering effects not existing in classical optics. Dielectric nanoscale structures are supposed to complement or even replace several plasmonic components in a range of potential applications. Furthermore, many concepts which had been developed for plasmonic structures, but fell short of their potential due to high losses of metals at optical frequencies, can now be used based on low-loss dielectric structures [8].

It's supposed that highly efficient all-dielectric metasurfaces with the extraordinary capability of polarization control can be commonly applied in areas of polarization detection and imaging, data encryption, display, optical communication and quantum optics for ultracompact and miniaturized optical systems realization [9]

Deep learning (DL) is a subcategory of machine learning (ML) which is based on layered structures described as artificial neural networks (ANNs). ANNs derive their name from the neural structures found in biological beings. This structure can be mathematically emulated as a node, denoted as a neuron, which may contain many input and output connections with correlated weightings. These neurons have a non-linear activation function that serves to map the inputs to an output and provides the switching behavior similar to that in biological neurons. These neurons are packed into layers which are connected to successive layers. The functionality of this is to construct a necessarily deep neural network such that any arbitrary function would be estimated. At the same time, the higher the ANN complexity the larger datasets is required for suitable prediction accuracy. ANNs can be considered as a mapping between input and output spaces which can be arbitrarily defined. For different tasks, ANNs can have complicated structures. The

dataset features are automatically learnt to set up the desired mapping from input to output. To perform a given task, the DL models should experience a process known as training [10].
Training a model requires the introduction of the so-called loss function, that provides feedback on the difference between the real output (or "ground truth") and the output predicted by the network for the same given input data. Training the ANN intends to minimize the loss function by adjusting the weight values at each layer. These tasks are commonly accomplished through some form of stochastic gradient descent which may be done effectively over the network with backward propagation [11]. The training is labeled complete when the model can predict the output with some required quality metric. After the training, the ANN can accurately map the input to the wanted output, implying that it has "learned" the necessary mapping from the given data. It should be known that this mapping is not essentially unique while differences in training procedure may lead to a failure to converge. Generally, a dataset is divided into training and validation sets. Due to high dimensional networks structure, over-fitting possibly occurs which should be mitigated. Over-fitting can be examined through the loss function applied to validation set. When the model is trained and over-fitting is overcome, the model considered to be capable of generating an output based on a sample input. This supposes that the training data provided is characteristic of the problem that one is trying to learn [12].
One of the major challenges of ML is the amount of data needed for the training procedure, which is typically determined by the complexity of the problem.
DL is useful for tasks that require repeated resolution with different parameters or for creating complex feature extraction tasks. In photonics, ML is mainly used for forward and inverse design. Forward design predicts physical responses (e.g., scattering spectra, polarization) for a given structure using tools like T-matrix calculations and full wave simulations to solve Maxwell's equations. While ML can serve similar purposes, its greatest advantage lies in inverse design problems, where it determines structure parameters for a desired response. DL supports this through surrogate modeling, offering data-driven approximations instead of simulations [13].
Surrogate models (SMs) are used to replace expensive simulation models of engineering problems. Although computers are becoming faster and more powerful, the demand for computational complexity is still outpacing the improvements in computer power and speed. Additionally, using computer simulations can be challenging due to their high fidelity, regardless of how fast or powerful computers are. Even methods like parallel computing, where many calculations or processes are executed simultaneously, do not fully address these issues [14].
Surrogate models trained on limited data accurately predict unit cell properties and speed up microscopic optimization. These models replace full-wave simulations to quickly predict meta-atom properties [15].
In previous work, deep learning has been utilized in metasurface design and response verification. CHRISTIAN et al. have demonstrated modeling of complex all-dielectric metasurface systems with deep neural networks achieving an average mean square error of only 1.16×10^{-3} and is over five orders of magnitude faster than conventional electromagnetic simulation software [16]. A data preprocessing approach based on the governing laws of the physical problem to eliminate dimensional mismatch between a high dimensional optical response and a low dimensional feature space of metasurfaces was proposed by Ibrahim et al. They trained forward and inverse models to predict optical responses of cylindrical meta-atoms and to retrieve their geometric parameters for a desired optical response, respectively. Using their inverse model, they designed and demonstrated a focusing meta lens as a proof-of-concept application [17]. A deep learning-based metasurface/meta-atom modeling approach was introduced by SENSONG et al. to significantly reduce the characterization time while maintaining accuracy. Based on a convolutional neural network (CNN) structure, the proposed deep learning network was able to model meta-atoms with nearly freeform 2D patterns and different lattice sizes, material refractive indices and thicknesses [18]. To reach the highest working frequency for training the DNN, Fardin et al. have considered 8 ring shaped patterns to generate resonant notches at a wide range of working frequencies from 4 to 45 GHz. They proposed two network architectures. In one architecture, they restricted the output of the DNN, so the network can only generate the metasurface structure from the input of 8 ring shaped patterns. This approach drastically reduces the computational time, while keeping the network's accuracy above 91%. They showed that the

model based on DNN can satisfactorily generate the output metasurface structure with an average accuracy of over 90% in both network architectures [19]. Xiaoshu et al. used deep learning methods to build a metamaterial database to achieve rapid design and analysis methods of metamaterials. They proposed a method to calculate the electromagnetic properties of metamaterials using DNNs. Effectively simulate the electromagnetic properties of periodic metamaterial structures [20]. VLAD et al. proposed an alternative data-free DL method using a physics-informed neural network (PINN) to enable more efficient computation of light diffraction from 3D optical metasurfaces, modeling of corresponding polarization effects, and wavefront manipulation. Once trained, the PINN-based electromagnetic field (EMF) solver simulates light scattering response for multiple inputs within a single inference pass of several milliseconds. This approach offers a significant speed-up compared to traditional numerical solvers, along with improved accuracy and data independence over data-driven networks [21].
In this paper, we have rebuilt the metasurface grating structure in [22] and used the surrogate model and DNN built-in COMSOL Multiphysics software, to optimize geometrical dimensions instead of the Monte Carlo optimization method used by Baki and Tawfeeq [22], to improve the performance by obtaining higher polarization extinction ratio (ER). Thus, improving its capability to function as a polarization modulator that is used in QKD systems. Simulation results of the obtained design show excellent extinction ratio of the polarizer. Thus, by utilizing COMSOL Multiphysics Surrogate model deep neural networks can help in optical component design improvement over conventional design methods.

2. Theory

DL ANN consists of an input layer, hidden layers and an output layer, as illustrated in Figure 1. Each layer is made of multiple nodes, those are fully or partially connected to the subsequent layer nodes. Each node has weight, that is tuned based on training. Biased parameter is added to the connection between two nodes too. The output $\boldsymbol{y_i}$ is a function of node input $\boldsymbol{x_i}$, weight $\boldsymbol{w_i}$ and bias $\boldsymbol{b_i}$, as in the following equation [23]:

$$y_i = \sum(x_i - w_i) + b_i \quad .... \quad (1)$$

In a supervised NN learning algorithm, input data comes with corresponding labels. The training process compares predicted results with these labels, continuously optimizing the network for better performance. It learns the relationships between metasurface structures and optical responses to perform specific optical functions. One of the main and fundamental supervised ANN algorithms is the multilayer perceptron (MLP) shown in Figure 1 [23].

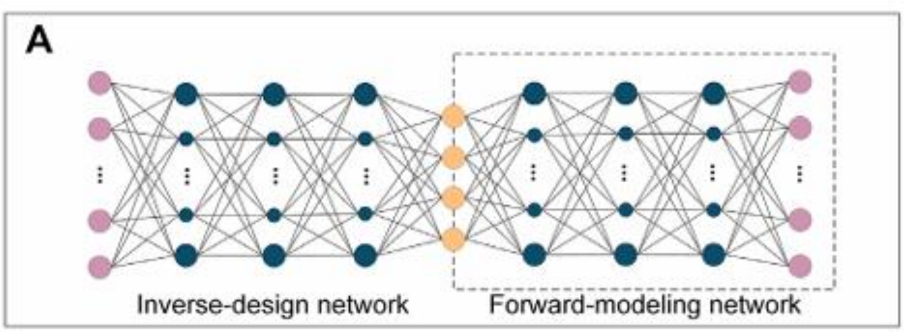

Fig. 1: Schematic illustration of typical deep learning model algorithm multiple perceptron [23]

The MLP is a key model in deep learning, forming the basis of all other ANNs. It links inputs to outputs through hidden layers with nonlinear activation functions. This model optimizes many parameters, allowing it to learn complex, nonlinear relationships in optical data. In training, a cost function based on variance or cross entropy is defined, and weights are adjusted using back propagation to minimize this cost. Then, target optical functions like scattering spectra are fed into the network to predict photonic structures. Adding more hidden layers increases feature learning and accuracy but can lead to over-fitting. The tandem network model solves non-uniqueness by combining inverse-design and forward-modeling networks, as shown in Figure 2 [24].

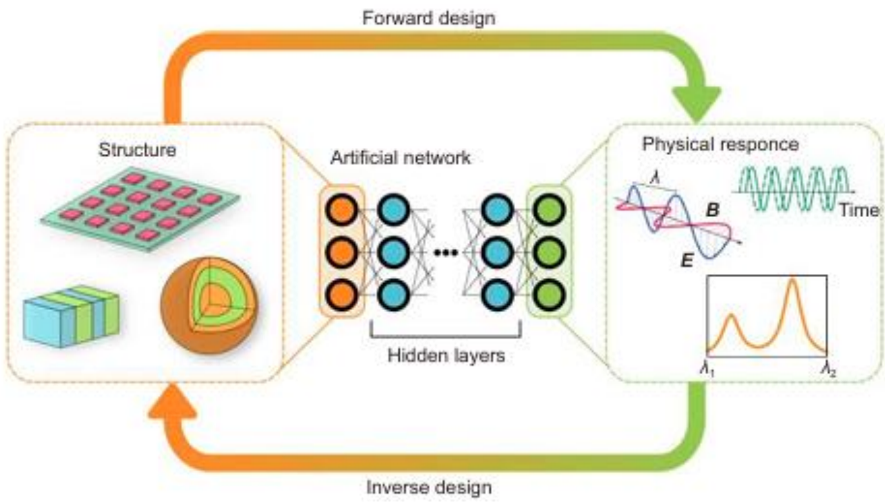

Fig. 2: Inverse and forward designs based on DL techniques [24]

2.1 Metasurface Polarizers

Metasurfaces generally consist of subwavelength structures (meta-atoms) arranged in a 2D plane. By adjusting the shapes, sizes, orientations, or positions of meta-atoms, a phase gradient can be introduced at the interface to mold the optical wavefront as needed. In addition to phase manipulation, metasurfaces leverage strong light–matter interactions at the subwavelength scale to regulate light across various degrees of freedom (DoFs) such as amplitude, frequency, chromatic dispersion, and polarization, using mechanisms like electric dipole resonance, magnetic dipole resonance, or guided mode resonance [9] [25] [26].
Polarization manipulation at the subwavelength scale is a unique capability of all-dielectric metasurfaces (ADMs), achieved by engineering the anisotropy of the media in contrast to traditional refractive and diffractive optical components. ADMs can be engineered to have much higher refractive index contrasts by introducing asymmetric meta-atoms compared to the principal refractive indices along two orthogonal axes (extraordinary and ordinary) difference in natural materials. Meta-atoms that are designed as birefringent elements can be used to achieve subwavelength polarization control for applications such as polarization conversion, polarization-dependent multiplexing, and complex vector beams. Combining these capabilities with phase and amplitude regulation allows for the realization of more complex functions [9] [25] [26].
In QKD systems, such as, the BB84 protocol two basis sequences are used, i.e. rectilinear and diagonal. The rectilinear basis includes horizontal 0° and vertical 90° polarization, while the diagonal basis has 45° and 135° polarization states. To generate these polarization states in the transmitter, optical polarizers are needed. With the high transmittance, high extinction ratio, compactness and integrability in optics, compared to bulk polarizers, metasurface polarizers are used in QKD transmitting systems [1] [2] [3] [27].

2.2 Deep Learning for Metasurface Structure Design

Metasurface optics have rapidly advanced over the past decades, demonstrating strong capabilities in controlling light-matter interactions. Recently, deep learning has revolutionized this field [23]. Traditional design methods, such as trial-and-error, parameter sweeps, and optimization algorithms, require extensive computational resources and time-consuming simulations. These simulations must be repeated if design requirements change, limiting user focus on actual needs. To address these issues, deep learning offers a faster, more efficient, and automated design approach [19].

3. Methodology

Over the past two decades, the explorations of metasurfaces have led to the discovery of exotic light–matter interactions, such as anomalous deflection, asymmetric polarization conversion and wave-front shaping. An inverse metasurface design is taking place by providing the structure optical response vs. its geometric parameters as a dataset to NN, the network can be trained to learn the relationship between the input and output [23] [19].

Nanowire periodic structure lattice of the metasurface grating polarizer is designed in the visible region [22]. Based on the effect of guided-mode resonance. Guided-mode resonance involves structures composed of a substrate, a waveguide layer, and a grating layer. When illuminated by an incident light beam, a portion of the beam is directly transmitted through the structure while another portion is diffracted by the grating and trapped within the waveguide layer. Subsequently, some of the trapped light is rediffracted, causing destructive interference with the transmitted part of the light beam. At specific wavelengths and angular orientations of the incident beam, the structure resonates, resulting in complete interference and no transmission of light. The critical factor is the relative phase shift between the incident and diffracted waves, leading to destructive interference. Figure 3 illustrates this process. The grating layer (layer 2), assumed to be infinitely thin, is positioned at the interface between the high refractive index waveguide layer and the surrounding medium. Most of the incident plane-wave, denoted by t, is transmitted through the structure as b. The grating diffracts a small fraction of the incident plane-wave into the first-order wave [28].

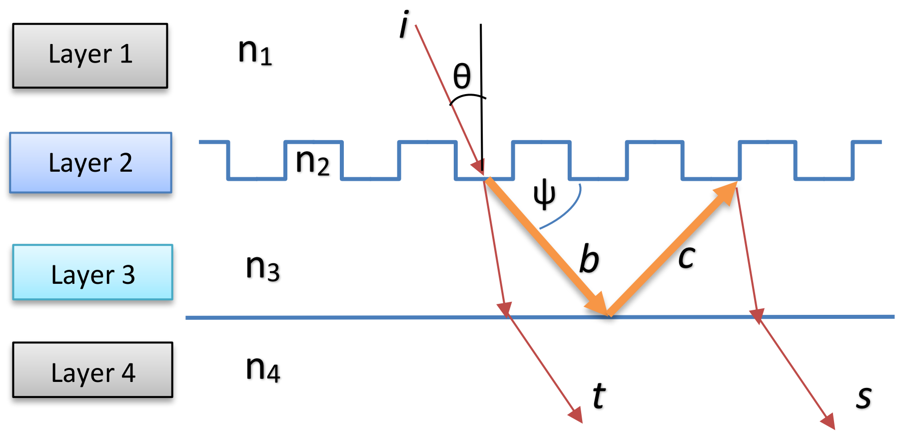

Fig. 3: Basic geometry of grating waveguide structure and relevant interference waves. Transmitted wave t and diffracted wave S originating from the incident wave i destructively interfere at resonance [28].

Here in this work, the metasurface structure passes the TM polarized light and blocks the TE one. Grating structure dimensions must be designed to ensure having the best polarizer performance, i.e., high ER can be obtained [22]. Hereby, deep learning neural networks algorithms can be utilized to perform dimensions optimization.

Then by applying a condition to restrict the required response, i.e., max$|T_{TM}|$ and min$|T_{TE}|$ at a specific wavelength, a linearly polarized light with maximum extinction ratio ER can be obtained as in Eq. (2) [22]. Thus, the trained network can propose the optimal geometrical dimensions of the structure which meet the requirements.

$$ER = \frac{T_{TM}}{T_{TE}} \quad .... \quad (2)$$

The structure in [22] consists of TiO_2 grating on a SiO_2 substrate of 1000 nm thickness. TiO_2 is chosen as the base material because it exhibits no loss $\kappa \approx 0$ and high index of refraction for strong light-matter interactions at visible wavelength spectrum [29]. The grating is covered by SiO_2 as in Figure 4, was built and simulated using COMSOL Multiphysics software as shown in Figure 5. The refractive indices of TiO_2 and SiO_2 are 2.5824 and 1.4570 respectively at $\lambda = 632$ nm.

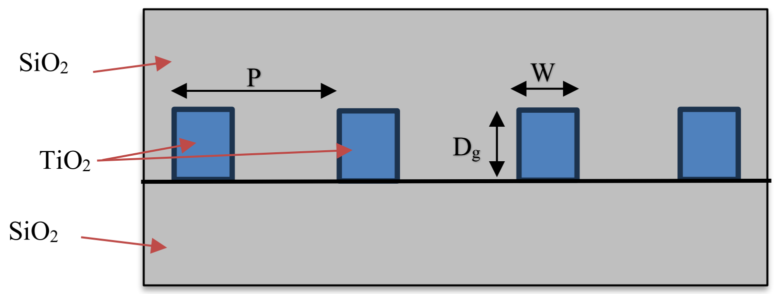

Fig. 4: Metasurface grating structure

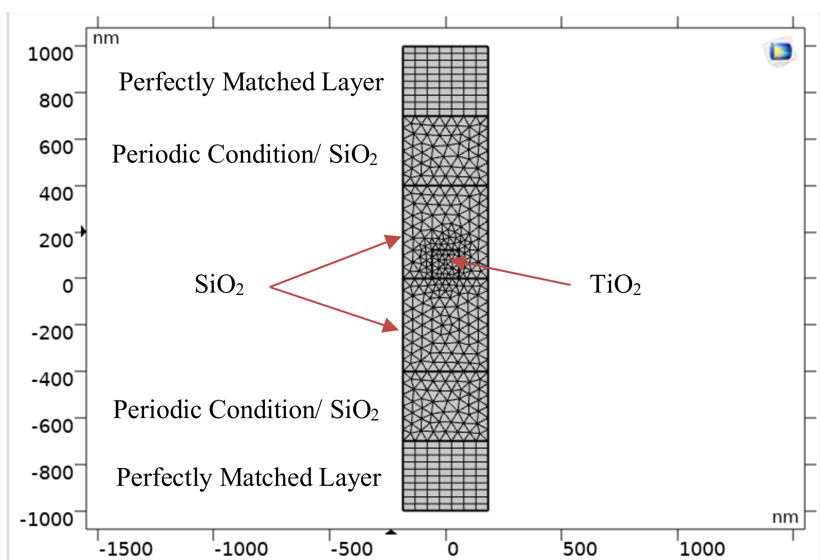

Fig. 5: Grating structure unit mesh configuration

Deep neural network, illustrated in Figure 6, was used to optimize the geometrical structure dimensions such as grating thickness D_g, grating period P and fill factor FF which is the ratio of grating width W to the grating period P. Thus, $FF = W / P$.

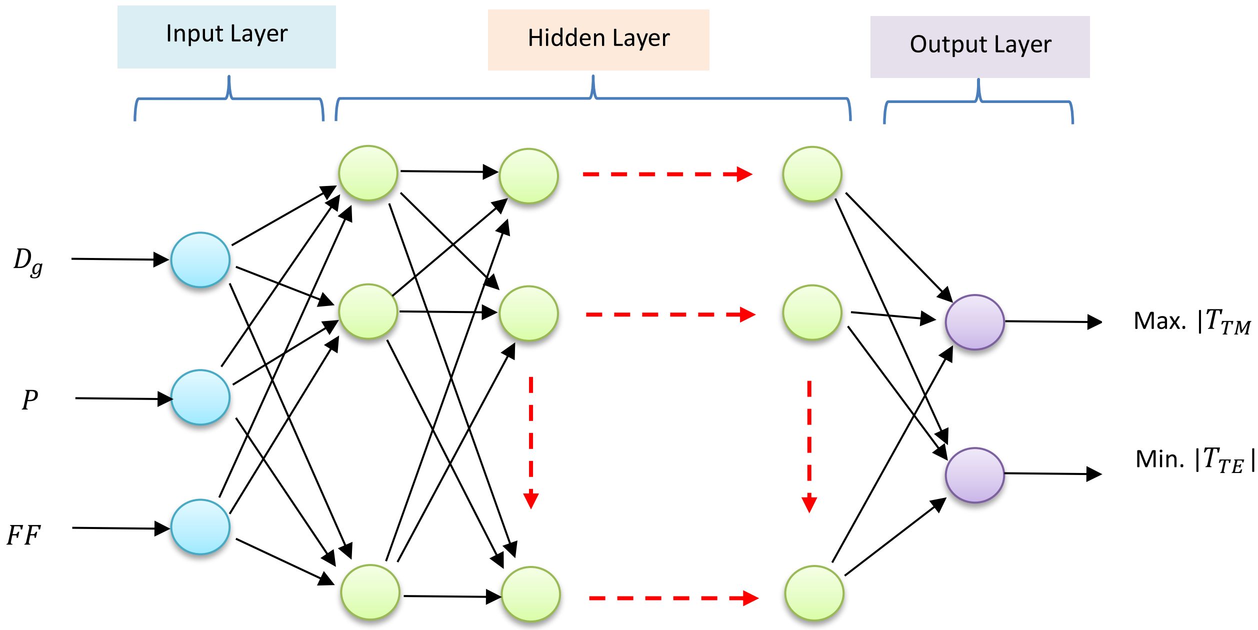

Fig. 6: ANN structure of the used model

Instead of Monte Carlo optimization method that was used in [22], where $ER = 1800$ was obtained in [22], the Surrogate model, a COMSOL Multiphysics software built-in tool, has been used to build and train an ANN with the dataset generated by specifying the input parameters limits and wavelength range, as listed in Table 1. The Surrogate model was trained on simulation data generated from a parametric sweep of structure geometry (P, D_g and FF, in addition to λ) to simulate the response (T_{TE} and T_{TM}), and was fed directly to DNN. For validation, 20% random samples (not used for training) of generated dataset were used.

Table 1. Surrogate Model Parameters Limits

Parameter	Lower limit	Upper limit
D_g	100 nm	390 nm
P	200 nm	400 nm
FF	0.1	0.9
λ	400 nm	800 nm

After execution of the model training, optimal structure dimensions were obtained that meet the output condition for higher ER. The loss function used to evaluate the learning capability of the neural network is calculated using mean square error MSE as the loss function (L), defined as in Eq. (3) [12]:

$$L(w_i, b_i) = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2 \quad \ldots\ldots \quad (3)$$

Then the whole wavelength range, 400- 800 nm, $\boldsymbol{T_{TM}}$ and $\boldsymbol{T_{TE}}$ responses were simulated to calculated $\boldsymbol{ER}$ using the obtained structure dimensions. The process was repeated, as illustrated in the block diagram shown in Figure 7.

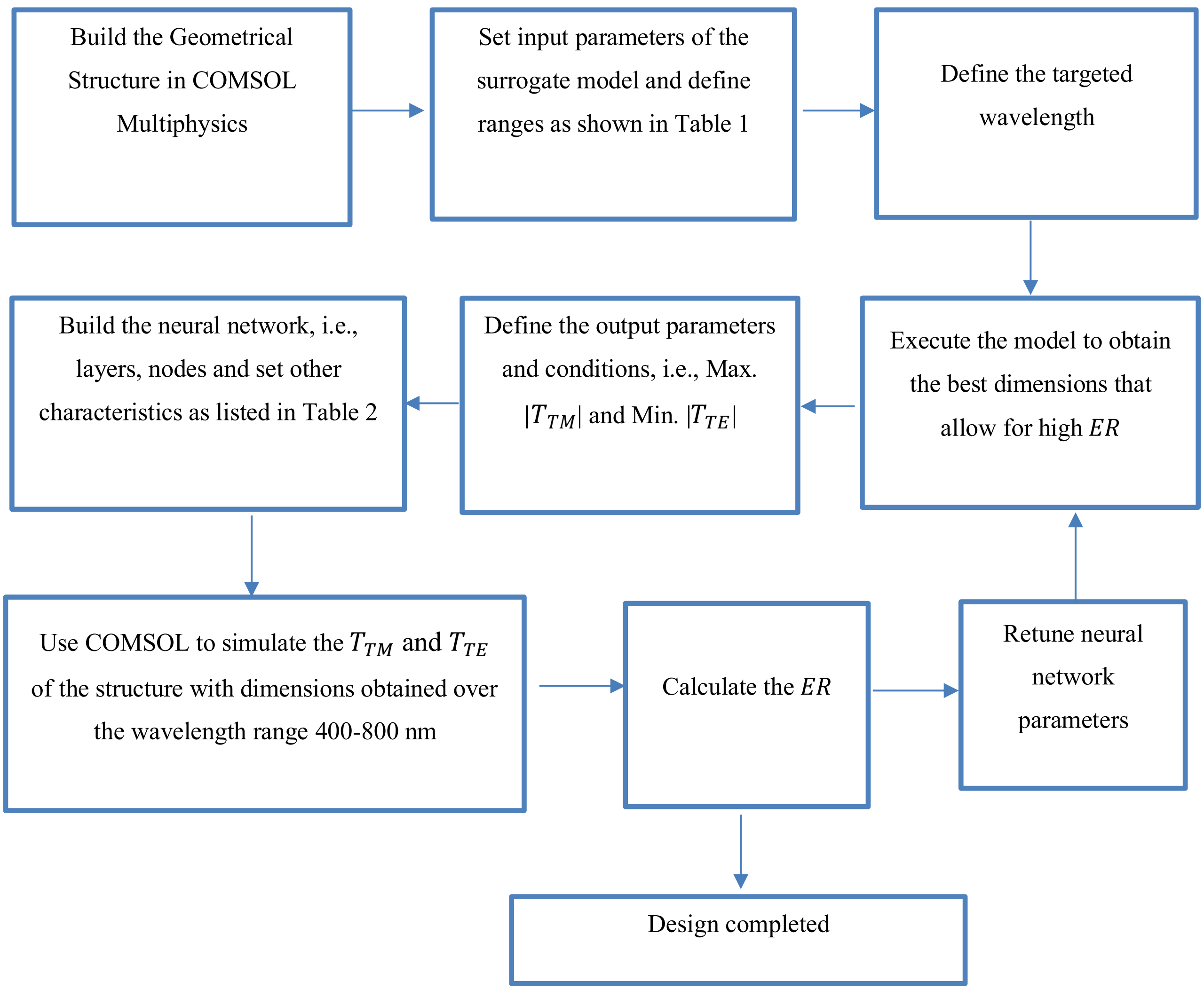

Fig. 7: Process block diagram

Table 2 Neural Network Parameter Setting

Parameter	Value	Description
Number of input nodes	3	Number of nodes of Neural network input layer, i.e. input parameters D_g, P and FF
Number of layers	10	Number of layers in Neural Network
Number of nodes per layer	512	Number of nodes per each hidden layer in neural network
Epoch size	1000	Determines how many times the model sees the entire dataset
Batch size	128	the size of the data subset passed through the network before the model's internal parameters are updated
Number of input points	500	Number to train the surrogate model to a sufficient degree of accuracy
Activation function	ReLU	Rectified linear unit
Output layer activation function	Linear	
Optimizer	Adam	Optimizer is the element that fine-tunes a neural network's parameters during training
Loss function	MSE	Measures how good a neural network model is performing a certain task
Validation	20%	random samples of dataset unused for training.
Number of output nodes	2	Number of nodes of Neural network output layer, i.e. TM and TE

4. Result and discussion

Based on block diagram illustrated in Figure 7, collected results were compared to tune the ANN parameters. Optimal obtained parameters were set for the final results, as illustrated in Table 2, based on the assessment of the training progress of the prediction, it can be noticed that validation loss did not drop similarly as much as the training loss curve did, as shown in Figure 8. This may indicate a kind of overfitting of ANN. Although, several tuning processes were made to NN parameters that improve the curve, yet difference is distinguished. However, the resulting performance parameter ($\boldsymbol{ER}$) showed excellent results. Sample results of tuning process are shown in Figure 9. The higher obtained $\boldsymbol{ER}$ was considered as the optimal design of the grating metasurface as shown in Figure 10, while EM field distribution for both $\boldsymbol{T_{TM}}$ and $\boldsymbol{T_{TE}}$ are plotted as shown in Figure 11.

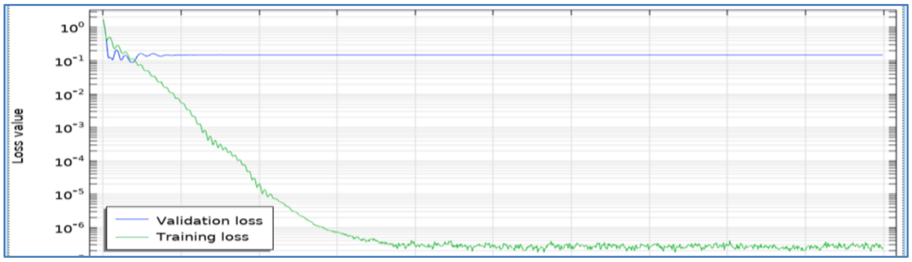

Fig. 8: Training progress graph of ANN

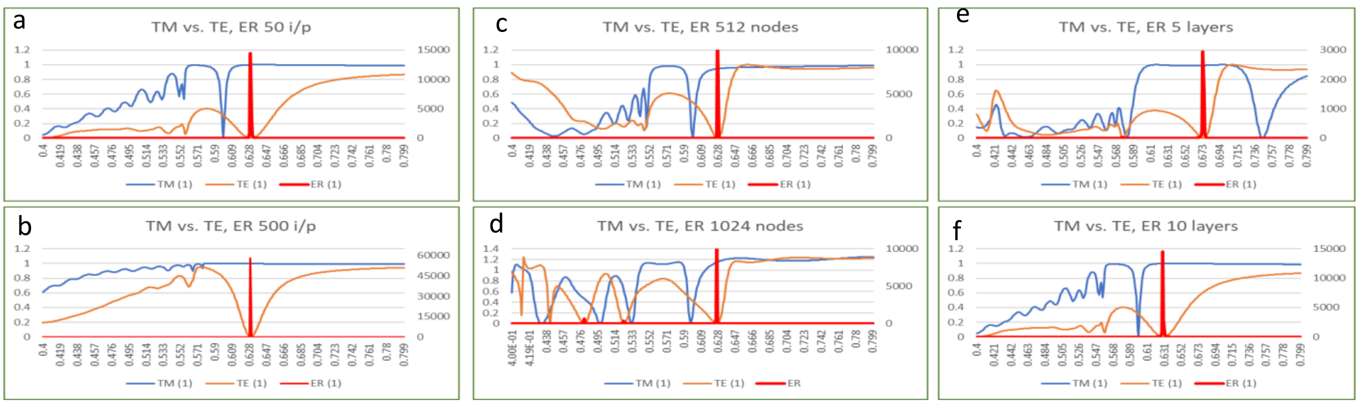

Fig. 9: Plot of T_{TM}, T_{TE} and ER vs. wavelength for different Surrogate Model parameter tuning samples. a and b, different inputs number. c and d, different hidden layers' number of nodes. e and f, different number of hidden layers.

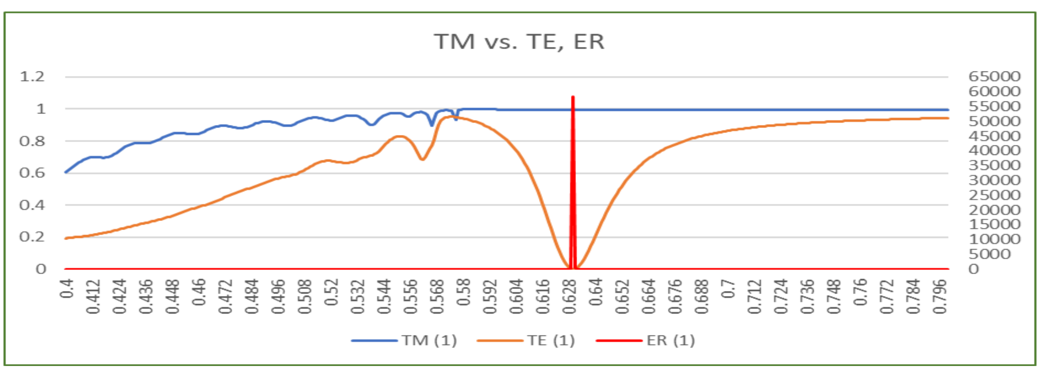

Fig. 10: Metasurface grating structure response based on the optimal Surrogate model proposed dimensions

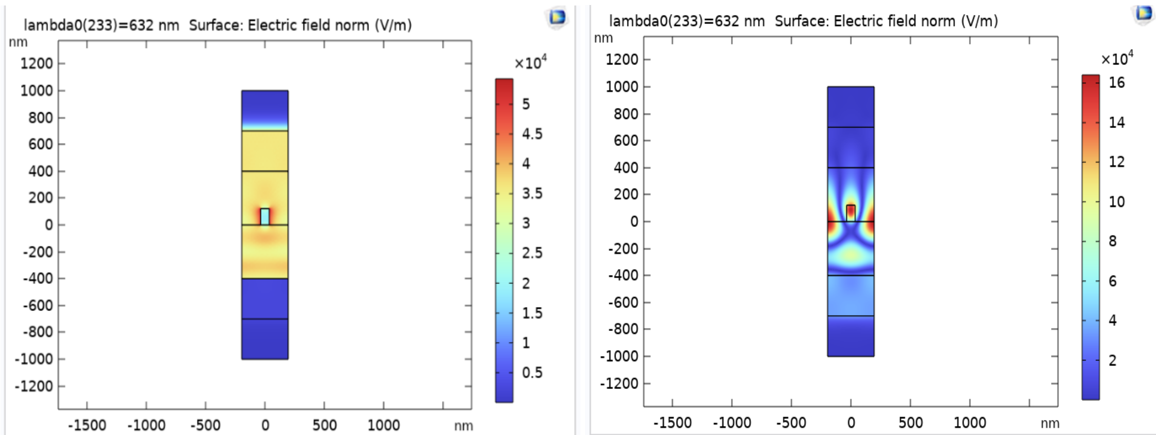

Fig. 11: The electric field distribution of the Surrogate metasurface grating structure. (a) T_{TM} (b) T_{TE}.

The result from COMSOL Multiphysics simulation is consistent with the predictions of the DL Surrogate model which validates the accuracy of the approach used.
Surrogate model and ANN proposed the dimensions, $\boldsymbol{D_g} = \mathbf{121.71}$ nm, $\boldsymbol{FF} = \mathbf{0.18302}$ and $\boldsymbol{P} = \mathbf{390.83}$ nm, as the optimal grating structure at $\lambda = \mathbf{632}$ nm, to achieve high $\boldsymbol{ER}$.
Optical response of the metasurfaces grating was simulated using the COMSOL Multiphysics over the wavelength 400-800 nm, resulting into an $\boldsymbol{ER} \approx \mathbf{60000}$, at the wavelength of interest, as illustrated in Figure 10, compared to 1800 using Monte Carlo optimizer in [22]. The response $\boldsymbol{T_{TM}}$ and $\boldsymbol{T_{TE}}$ of the polarizer grating structure are simulated with dimensions change tolerance of ±10% to demonstrate the fabrication error. Results show good tolerance for $\boldsymbol{D_g}$, good tolerance for $\boldsymbol{P}$ and very good tolerance for $\boldsymbol{FF}$ as illustrated in Figure 12, a, b and c respectively.

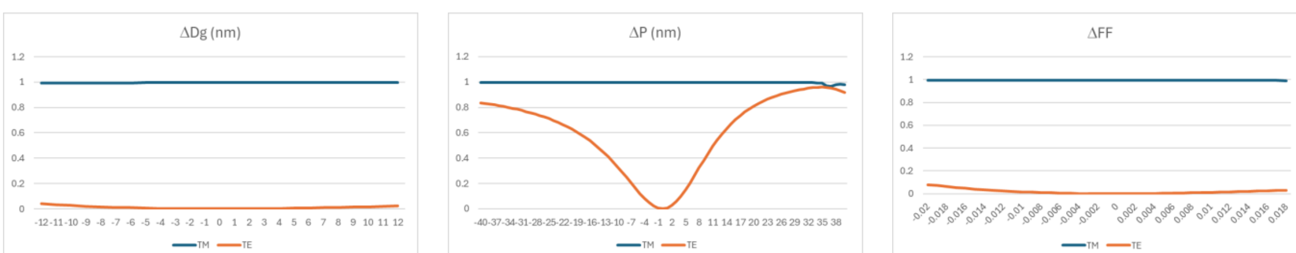

Fig.12: Structure dimensions response with ±10% tolerance. (a) grating thickness D_g (b) grating period P (c) fill factor FF.

5. Conclusions

Utilizing the DL technique, Surrogate model, and DNN built-in COMSOL Multiphysics software, have been used to optimize dimensions of TiO_2 metasurface grating structure, to obtain high quality polarizer with high $\boldsymbol{ER}$ of ≈ 60000 at $\lambda = \mathbf{632}$ nm, in visible spectral region. Thus, by using the Surrogate model and DL, the design process results were highly improved compared to conventional iterative optimization techniques such as Monte Carlo used in [22]. Hence, this polarizer can be used for photon polarization state encoding in QKD systems.

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تحسين الأداء لمستقطب محزز من الأسطح الفعالة باستخدام التعلم العميق لمنظومات توزيع المفتاح الكمومي

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الخلاصة: المستقطبات المصنوعة من الأسطح الفعالة هي مكونات بصرية أساسية في دوائر البصريات المتكاملة الحديثة وتلعب دورًا حيويًا في العديد من التطبيقات البصرية بما في ذلك منظومات توزيع المفتاح الكمومي في التشفير الكمومي. ومع ذلك، يعتمد التصميم العكسي للمستقطبات المصنوعة من الأسطح الفعالة ذات الكفاءة العالية على التخمين الجيد للأبعاد الهيكلية بناءً على الاستجابة البصرية المطلوبة. يمكن لشبكات التعلم العميق أن تساعد بشكل فعال في عملية التصميم العكسي، مما يقلل من الوقت والمتطلبات المتعلقة بالمحاكاة، بينما يمكن تحقيق نتائج أفضل مقارنة بطرق التحسين التقليدية. وبالتالي، يمكن استخدام نموذج Surrogate والشبكات العصبية العميقة في برنامج COMSOL Multiphysics لتصميم هيكل مستقطب محزز من الأسطح الفعالة مع نسبة فصل عالية تبلغ حوالي 60000 عند طول موجي مقدا ره 632 نانومتر ضمن الطيف المرئي.