# Designing rectangular surface Bragg gratings using machine learning models

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***Abstract*—In this paper, we demonstrate a possibility to predict the characteristics of semiconductor-based Bragg gratings using machine learning methods. We perform 2D simulations of the Bragg gratings and calculate reflectance to create a database. With obtained data, we train ML models to predict the shape of the upper part of the main peak of reflectance. We compare the performance of the widely used neural network with various different models on our data and demonstrate the high accuracy of the optimized XGBoost method.**

***Index Terms*—Bragg gratings, FDTD simulations, machine learning, optimized XGBoost.**

## I. Introduction

State-of-the-art concepts for the realization of monolithically integrated ECDL (mECDL) include the distributed periodic Bragg-reflector structure. [1] In order to aid the mECDL design process specifically related to the surface periodic Bragg grating design, we use machine learning (ML) methods. We investigate the reflectivity spectrum, namely the central lobe in reflectance, using two-dimensional (2D) finite difference time domain (FDTD) methods.

Among various techniques to design surface Bragg gratings, brute force optimization of the main parameters is the very cornerstone of the design processes. However recently, more advanced optimization techniques [3] based on various statistical methods for the inverse design have been developed. These optimization techniques, whether brute force or more advanced optimization are very time-consuming for multi-dimensional parameter space, particularly if one uses the FDTD simulations. On the other hand the intuitive-driven parameters-based phenomenological models such as coupled mode theory [4] are less time-consuming but limited in their predictive power.

Here we take advantage of the predictive power of ML methods, combined with the accuracy of the FDTD simulations to design certain characteristics of rectangular surface Bragg gratings. In order to run thousands of 2D simulations for generating the database, we used a fully efficient and automated approach. We used various ML methods to compare their predictability on our small database. Artificial neural network (ANN), which is a deep learning model has been very successful in inverse design problems recently. In addition to ANN, we used various other ML methods for comparison. Deep learning models require large data, so we used other ML methods that are known to perform well on a small database, some of which are based on Scikit-learn library.

This work was supported by the VDI Technologiezentrum GmbH with funds provided by the Federal Ministry of Education and Research under grant no. 13N14906 and the DLR Space Administration with funds provided by the Federal Ministry for Economic Affairs and Climate Action (BMWK) under Grant No 50WK2272.

## II. Results and discussions

We consider a GaAs single-mode ridge waveguide. The grating is made as a set of periodic rectangular grooves. To perform a 2D simulation we consider a cross-section of the structure along the waveguide. (figure 1(a)) Details of the geometry are presented elsewhere [2].

Variations in Bragg gratings' depth, width and grating order in terms of their period are playing a major role in our reflectance spectrum. Therefore we created 2055 2D simulations by varying the width, depth, and grating order. Generating a 2D database allows us to create a larger database for which the data analyses are more informative due to the number of parameters. We focused on the main lobe of the reflectance as the optical response. It is worth noting that all FDTD simulations were done by an automated design script.

The depth and the width of the grating determine the amplitude and the bandwidth of the main reflectance peak. With an increase in the depth of the grating, the interaction of the optical field with the change in the refractive index of the grating becomes stronger. As a result amplitude of reflection is generally larger for deeper gratings. Similarly with an increase in the width (while it is still much smaller than the wavelength), the peak reflectivity amplitude also increases. The bandwidth of the main peak is usually determined by the length of the structure and the losses. An increase in the interaction of the optical field with the gratings generally increases radiative losses causing a small increase in the bandwidth. Grating order is a discrete parameter whose value is an integer in the range 6-10. It corresponds to the number of wavelengths that fit within a round-trip between two nearby grooves. In addition to some of the most common ML models for regression, we use more advanced techniques, such as optimized extreme gradient boosting (XGBoost) and ANN. The ML methods that we compare in this study are polynomial($m^{th}$-degree) regression, support vector regression

(SVR), decision tree (DT) (with optimized depth), and K-nearest-neighbor, KNN (with optimized number of nearest neighbors, nn), XGBoost and optimized ANN. To begin, we

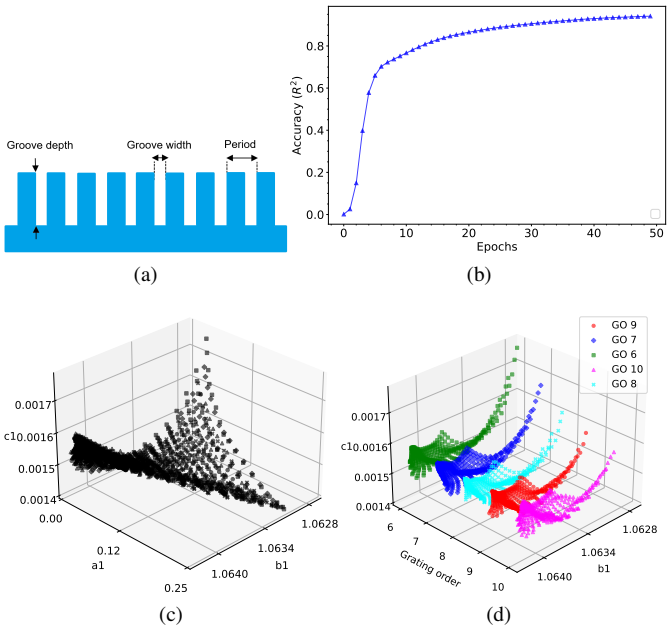


Fig. 1: (Colour online) (a) Shows the side view of the geometry (b) shows the accuracy of the optimized ANN model on the training set as the number of epochs progresses. (c, d) Show the results of K-means clustering model in correctly clustering the data based on the grating order (a1, b1, c1 are the Gaussian fit parameters according to $f(x) = a_1 exp[-((x-b_1)/c_1)^2]$).

divide our data set into two training and test sets. We use 75% of the data for training and the remaining 25% for testing. The testing set is kept untouched throughout the training procedure to ensure no information leakage. Since the actual values of the data are in various ranges with different distributions (amplitude is in the range between 0 and 1, while the bandwidth is of the order of $10^{11}$, and depth and width are of the order of $10^{-8}$), we standardize the data to reduce model sensitivity to various scales in the data. Standardization is applied to all the features except the grating order. Since this feature is a discrete value (between 6-10), we apply the One-Hot-Encoder approach. This approach has a similar purpose as standardizing the data but instead is used to convert categorical data into a binary vector. After preprocessing step we apply various ML methods to our data.

Figure 1(b) shows how the accuracy of our ANN model improves as the number of epochs progresses. This graph is done after the hyperparameters have been optimized. Figure 1(c, d) shows how our ML model is able to cluster the data. If we look at panel 1(c), we see that the output values are very close to one another. Panel 1(d) shows the plot in which we applied the K-means clustering method to illustrate the clustering based on the grating order. K-means clustering partitions data into K clusters in a way that data points in the same cluster are similar. When we plot panel 1(c) again, with the a1 axis replaced with grating order (1(d)), it is clear that the data is categorized correctly.

TABLE I: Performance comparison between various models, with width, depth, and grating order as input and upper part (2/3) of the central lobe in reflectance as output.

| ML models | training set | | test set | |
|---|---|---|---|---|
| | $R^2$ | $\sigma$ | $R^2$ | $\sigma$ |
| polynomial ($m$ = 5) | 0.980 | 0.004 | 0.980 | 0.002 |
| SVR | 0.957 | 0.012 | 0.958 | 0.007 |
| DT (depth 9) | 0.955 | 0.007 | 0.958 | 0.004 |
| KNN (nn=2) | 0.984 | 0.006 | 0.987 | 0.003 |
| optimized XGBoost | 0.995 | 0.002 | 0.997 | 0.001 |
| optimized ANN | 0.941 | 0.006 | 0.949 | 0.007 |

The table I represents the performance of each model on width and depth and grating order being the input and the upper part (2/3) of the reflectance spectra being the output. We fit this part of the spectra with a Gaussian function and used the fit parameters as the output. The results in this table are carried out for 10-fold cross-validation with $n$ = 3 times repeated, to ensure that they are indeed correct. The figure of merit, $R^2 = 1 - (\sum_i (y_{true} - y_{pred})^2 / \sum_i (y_{true} - y_{mean})^2)$, is the accuracy measure in table I. The $y_{true}$ and $y_{pred}$ are the actual values of the target feature and the predicted values, respectively. The $R^2$ value of 1 is associated with a perfect prediction. $\sigma$ describes the standard deviation among the calculated $R^2$ values for all the folds and repetitions. We see from the table I that all the models perform well, while the performance of the deep learning model, ANN, is slightly worse than the others, even though we optimized the ANN hyperparameters. On the other hand, the best performance is achieved with optimized XGBoost.

## III. Conclusion

We demonstrated a possibility to predict the characteristics of semiconductor-based Bragg gratings by means of machine learning methods. We compared the performance of the widely used ANN with various different models on our data and demonstrate the high accuracy of the optimized XGBoost method.

## References


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