Apply Machine Learning Models and Reverse Engineering on Predicting Optical Properties of Semiconductor Bilayers

Vivian Hu & Xiyi Chen, Andre Schleife, Michal Ondrejcek, Erick Ivan Hernandez Alvarez

University of Illinois at Urbana-Champaign, University of Maryland, College Park

INTRODUCTION

Semiconductor nanocrystals play key roles in biomedical applications. These tiny light-emitting molecules are able to optically tag proteins for molecular imaging and targeted therapy. Therefore, intense amount of researches are done on changing the size and shape of these particles to tune for the desired optical properties.

Predicting Single Peak

The first goal this project focused on is predicting the wavelength of peak transmission and reflection of semiconductor bilayers using materials TiO2, HfO2, ZnO, AlAs, Ge, Si, and ZnS as the first layer (or incident layer) and second layer alternatively with thicknesses varying from 100 nm to 500 nm. In our models, four properties will be varied and used as input parameters: the type of material on the first layer (Material 1), the type of material on the second layer (Material 2), the thickness of Material 1 in nm, and lastly, the thickness of Material 2 in nm.

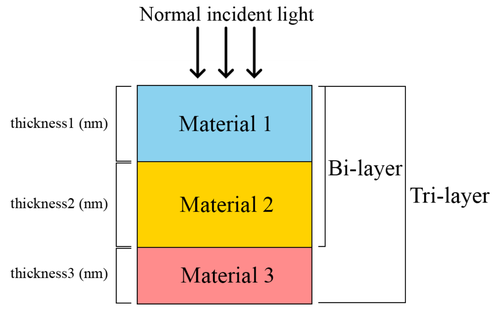
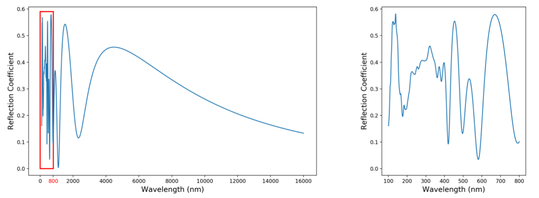


Figure 1: Schematic of the multilayer material systems studied in this work.

Entire Spectrum

The application of high throughput screening to the search for materials with specific optical properties is advantageous for the development of smart windows, or electrochemical films that respond to light signals to conserve resources. The design of these materials requires optimizing their optical responses, but standard computational methods for determining transmission and other property values requires solving Maxwell's equations, which is computational expensive when the materials design becomes complicated. In order to further decrease the cost of finding optimal materials combination, we propose an inverse materials design system that utilizes supervised machine learning to replace Maxwell's solver to predict the entire spectrum. We perform an experiment using materials TiO2 and HfO2. Once we have the model, a differential evolution algorithm is implemented to design systems with desired transmission spectrums.

METHOD



(a) Spectrum in 16,000 nm Wavelength Full Range

(b) Spectrum in Visible Range

Figure 2: (180 nm TiO2, 330 nm HfO2) Spectrum in 16,000 nm and 800 nm Wavelength Range

1. Single Peak

1.1 Linear Regression Model

Overall, we tried two different approaches for the Linear Regression Model:
1) Allow materials as the input parameters and build one giant model.
2) Build different models for distinct material combinations with thickness1 and thickness2 as the only parameters.

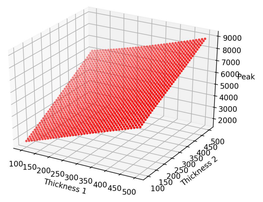


Figure 3: 3D Representation of the Linear Relationship between Thicknesses and Reflection Peak Position

1.2 Random Forest Model

The decision to use Random Forest Regression algorithm for this research is quite intuitive. Since there are only seven materials in our dataset and we observed that there are similarity in reflection/transmission for certain materials and thickness combination, it is reasonable to group several materials or thickness together in the first place to separate the similar combinations from other combinations and then find out the differences among the group.

2. Entire Spectrum

We use a Matlab based Maxwell solver to generate database. We selected the 200 - 900 nm visible wavelength range and 100 – 500 nm thickness range with an interval of 5 nm. The features include material thicknesses, combinations (in form of one-hot vector), and a particular wavelength value. The label to be predicted is the corresponding transmission value. All features are rescaled in between 0 and 1. The loss function used is Root Mean Square Error (RMSE).

We tried two different approaches to perform regression for the entire transmission spectrums. 10% of data is shuffled out for testing.

1) Random Forest: the remaining 90% data is used to for training. All hyper-parameters are tuned by performing grid-search with a 10-fold cross-validation.
2) Deep Learning: a stacked deep LSTM neural network is trained on 80% training data and 10% validation data. Hyper-parameters are tuned by trial and error. A 10-fold cross validation is performed. The final prediction is averaged on all 10 models.

To test the performance of our inverse design, a reasonable thickness range which the target thickness combination is likely to lie in is selected to build a candidate pool. The differential evolution algorithm goes through 1000 iterations, for each iteration, some new random or refined thickness combinations will be added in and unnecessary combinations will be removed. Finally, the materials combination with the lowest error was selected as the final solution.

RESULTS

1. Single Peak Model Comparison

Mean Absolute Error (MAE) in Peak Reflection Wavelength (nm)	Mean	Std	Max	Min
Linear Regression Model	77.204	65.453	4.139	221.338
Random Forest Regression Model	22.489	29.419	0.000	937.901

Table 1: Comparison of MAE differences for Two Models

2. Candidate Material Combinations

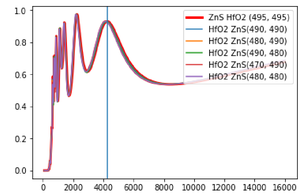


Figure 4:

[Good Match]

1st Layer: HfO2
2nd Layer: ZnS

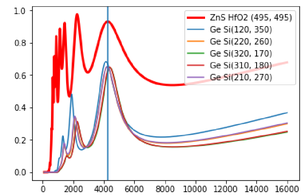


Figure 5:

[Peak Wavelength Position Match]

1st Layer: Ge
2nd Layer: Si

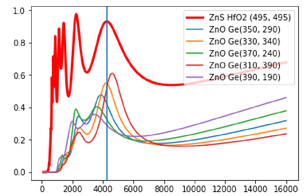


Figure 6:

[Bad Match]

1st Layer: ZnO
2nd Layer: Ge

3. Entire Spectrum Prediction

RMSE / Model	Mean (5-600nm)	Std (5-600nm)	Mean (100-500nm)	Std (100-500nm)
Random Forest	0.0825	0.0695	0.0063	0.0055
LSTM	0.0312	0.0584	0.0011	0.0003

Table 2: Comparison of Two Models of Transmission Spectrum Prediction

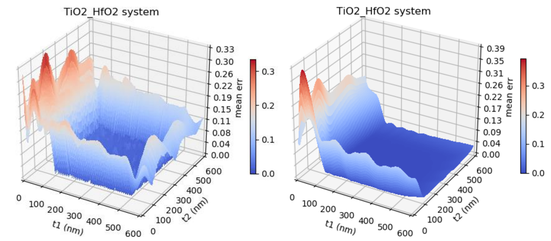


Figure 7: Comparison of Prediction Error between Random Forest (left) and LSTM (right) on TiO_2_HfO_2 system

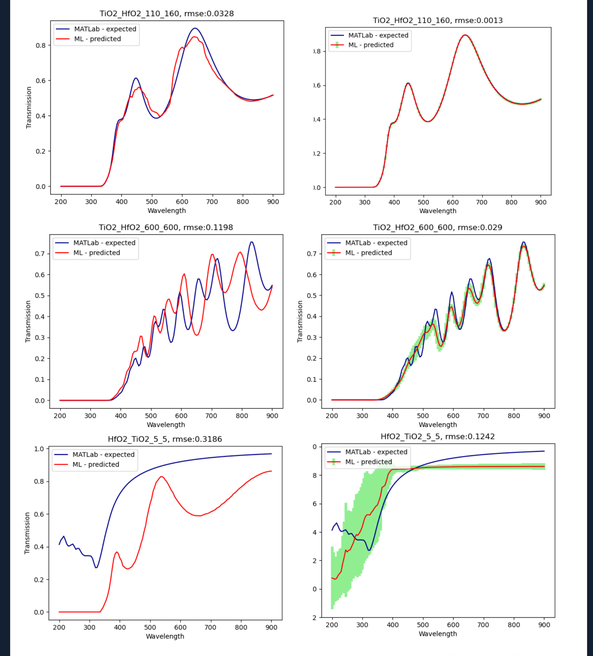


Figure 8: Comparison of performance between Random Forest (left) and LSTM (right) on both interpolative and extrapolative cases

Target Spectrum	LSTM	Random Forest
HfO_2_TiO_2_215_285_dense	0.0009	0.0057
TiO_2_HfO_2_530_520_sparse	0.0048	0.0487
HfO_2_TiO_2_30_75_sparse	0.0828	0.0980

Table 3: Comparison of RMSE of Inverse Design between LSTM and Random Forest Model

CONCLUSIONS

The Long Short-Term Memory deep neural network model is shown to have better performance than the Random Forest when predicting the entire spectrums. It produces smaller average and standard deviations on both interpolative and extrapolative test cases.

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