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Inverse Design of PbS Colloidal Quantum Dot Spectrally-Selective Photovoltaic Films

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Abstract: The inverse design of photovoltaic 2D photonic crystals using machine learning will be presented. The technique bypasses calculation of photonic bandstructure in favor of directly computing designer-friendly properties such as spectral transmission.

1. Introduction

Photonic Crystal (PhC) features have been used for a wide variety of optical components. The design of PhCs is typically done in the traditional computational sense: finite element or finite eigenmode methods are used to calculate photonic bandstructures, and these bandstructures are used to extract optical properties of the crystal. Forward optimization techniques such as gradient descent or interior point optimizations can then be used to solve for the optimal crystal structural parameters [1]. Recent advances in machine learning (ML) regression problems have led to the development of inverse design paradigms, where a crystal's desired optical properties are used as inputs and the crystal's physical parameters are back-propagated and extracted via a trained neural network (NN) [2, 3]. Here, we present the inverse design of photonic crystal slabs using materials with dispersive and absorptive (complex, wavelength-dependent) refractive indices, which are of great interest for energy harvesting systems such as multijunction solar cells and infrared sensors. This work highlights the use of NNs to design structured films of lead sulfide colloidal quantum dots (PbS CQDs) to tailor absorption and transmission spectra that can be optimized for applications in tandem solar cells or infrared sensing, in the regime where the PbS CQDs are absorptive. A NN model can be trained using a physics-based methodology such as the Fourier Modal Method (FMM) to produce high fidelity absorption and transmission spectra, and then deconvolved to inversely calculate the desired photonic crystal unit cells, as shown in Figure 1. Additionally, complex unit cells can be inferred through this method, as opposed to the limited traditional geometries, such as cylinder or hole arrays in a dielectric slab. This framework results in both faster design times as well as richer spectral selectivity, as the NN maps transmission and absorption spectra directly to complex unit cell geometries, which would not be computationally feasible to design with forward optimization techniques or structural search design paradigms.

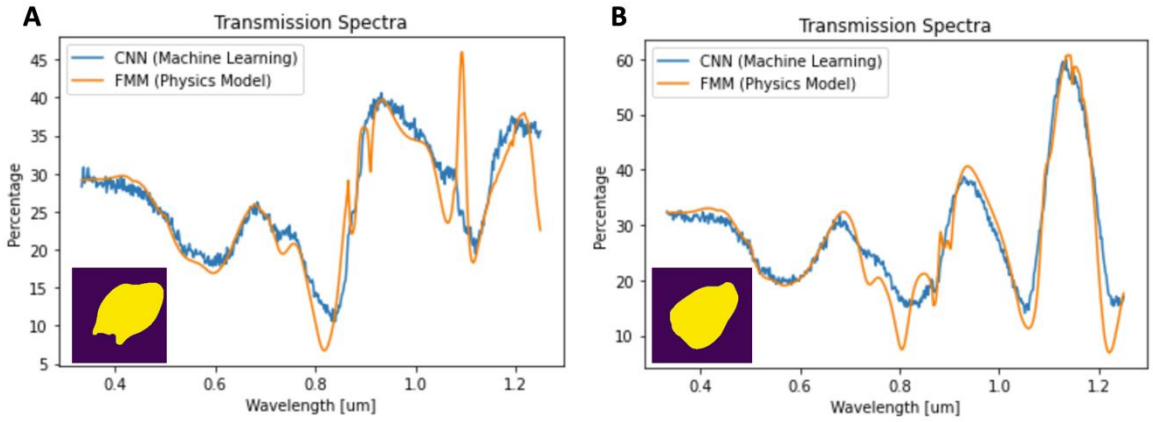

Figure 1: (a) FMM calculated spectra (orange) for a periodic lattice composed of unit cells of the arbitrary shape pictured in the inset (purple = air, yellow = PbS CQD film) used for NN training (blue). (b) Another example several epochs into NN training with the FMM spectra (orange) and NN spectra (blue) converging for the PhC geometry shown in the inset.

2. Results

The out-of-plane transmission, reflection, and absorption spectra of a PhC slab couple to the in-plane wave-guiding modes of the slab, and thus a PhC slab can be designed to create spectrally-selective films. Traditional methods such as finite-difference time-domain (FDTD) solvers have been used to calculate photonic bandgaps of 2D photonic

crystal slabs [4]. While optical properties can be extracted from the photonic bandstructure, optoelectronic designers are generally concerned with measurable thin film properties. The Fourier modal method (FMM) slightly alleviates this problem by calculating the out-of-plane spectra directly but is typically implemented for the forward problem. However, even using the FMM method, traditional parametric optimization techniques such as gradient descent typically result in reaching the boundaries of the search area. Weighting the figure-of-merit (FOM) to optimize absorption in the near-infrared - for example, if one is interested in optimizing the properties of the infrared cell of a multi-junction photovoltaic device - results in a maximally thick film composed primarily of the absorbing medium, whereas weighting the FOM to optimize transmission above the solar cell bandgap results in a slab that is as thin as possible, as would be expected from first principles given the materials' complex index models. We leverage FMM to generate training data for a convolutional neural network. Once converged, the trained neural network can then directly calculate the expected transmission spectra from an input geometry, without relying on the computationally expensive bandstructure calculation and extraction of spectra.

Figure 2 shows a comparison of traditional gradient-based optimization vs. the ML technique to generate a PhC unit cell to approach an ideal high-pass optical filter, useful for NIR solar cells in a tandem solar architecture. We note that the complex geometry that is inferred by the NN leads to better results, which could be of use for optoelectronic applications which target narrow spectral bandwidths or unusual optical spectra.

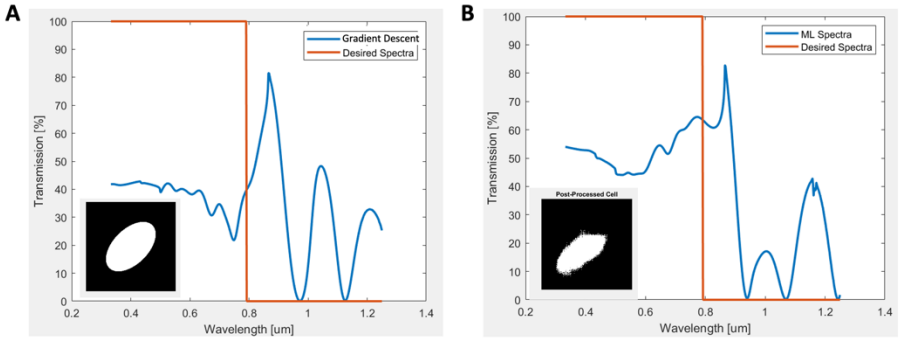

Figure 2: (a) A PhC unit cell generated by iterating through multiple geometries using gradient-descent based optimization while trying to match the calculated and desired spectra. (b) A unit cell generated by a trained convolutional and deconvolutional NN. The inset shows the unit cell geometry with the white representing the PbS CQD material, and black representing air.

The NN model takes in PhC unit cells and predicts their transmission and reflection spectra over a wavelength range of 333 nm to 1250 nm with a resolution of 500 data points. The NN model consists of a feature extraction component and a predictive component. The feature extraction component is a convolutional neural network (CNN) that takes in 2-D pixel values of the PhC unit cell, and it iterates the data through repetitional layers of convolution and max-pooling. The convolution portion applies a kernel with a specified depth to generate several filtered images equal to the depth of the kernel; the convolutional implementation is critical to keep extracted edges localized to the 2-D space in the image. Then, an activation function is implemented, and finally max-pooling is performed by extracting the maximum of every block of pixels to prevent over-fitting and reduce computation. Ultimately, the feature extraction portion is an abstraction of the input image that reduces the 2-D image to a 1-D vector. This vector becomes the input to the predictive component, which is a multi-layer and fully-connected deep neural network (DNN) that maps the abstract vector to final predicted transmission and reflection spectra output. This demonstrated inverse design method is a promising tool for designing spectrally-selective materials for photovoltaic applications.

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3. References

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