Effective and Equivalent Refractive Index Models for Patterned Solar Cell Films via a Robust Homogenization Method

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Abstract

Solar cells containing complex geometric structures such as texturing, photonic crystals, and plasmonics are becoming increasingly popular, but this complexity also creates increased computational demand when designing these devices through costly full-wave simulations. Treating these complex geometries by modeling them as homogeneous slabs can greatly speed up these computations. To this end, we introduce a simple and robust method to solve the branching problem in the homogenization of metamaterials. We start from the branch of the complex logarithm in the Nicolson-Ross-Weir method with the minimum absolute mean derivative in the low frequency range and enforce continuity. This is followed by comparing the reflectance, transmittance, and absorptance of the original and homogenized slabs. We use our method to demonstrate accurate and fast optical simulations of patterned PbS colloidal quantum dot solar cell films. We also compare patterned solar cells homogenized via equivalent models (wavelength-scale features) and effective models (sub-wavelength-scale features), finding that for the latter, agreement is almost exact, whereas the former contains small errors due to the unphysical nature of the homogeneity assumption for that size regime. This method can greatly reduce computational cost and thus facilitate the design of optical structures for solar cell applications..

Introduction

The full-wave simulations required to study 2D/3D structures such as photonic crystals, plasmonic structures, and textured surfaces are computationally costly. In this work, we homogenize patterned layers and reduce the problem to 1D, for which methods such as the Transfer Matrix Method (TMM) can be used. Once a homogenized model is produced, it can be reused in many simulations, reducing the computational cost drastically. We investigate the regimes:

- Effective models: inhomogeneity feature size $\ll \lambda$
- Equivalent models: inhomogeneity feature size $\approx \lambda$

Parameter Extraction Method

A popular homogenization method is the Nicolson-Ross-Weir (NRW) method, which starts from the S-parameters to obtain the complex refractive index of a corresponding homogeneous slab. The imaginary part is unique but the real part depends on a complex logarithm with multiple branches. The ambiguity of the branch index m results in a branching problem, which must be resolved. Our below method is more robust than taking the starting m as 0. Our method follows:

1. S-parameters obtained from Finite Difference Time Domain (FDTD) simulations.
2. NRW formulae to get complex refractive index.
3. Choice of branch with lowest absolute mean derivative across low frequencies, since many refractive indices behave this way
4. Continuity for the remaining frequencies.
5. Reflectance, transmittance, absorptance comparison.
6. Minimize mean square error between optical behavior of effective/equivalent model and simulated structure to obtain effective thickness.

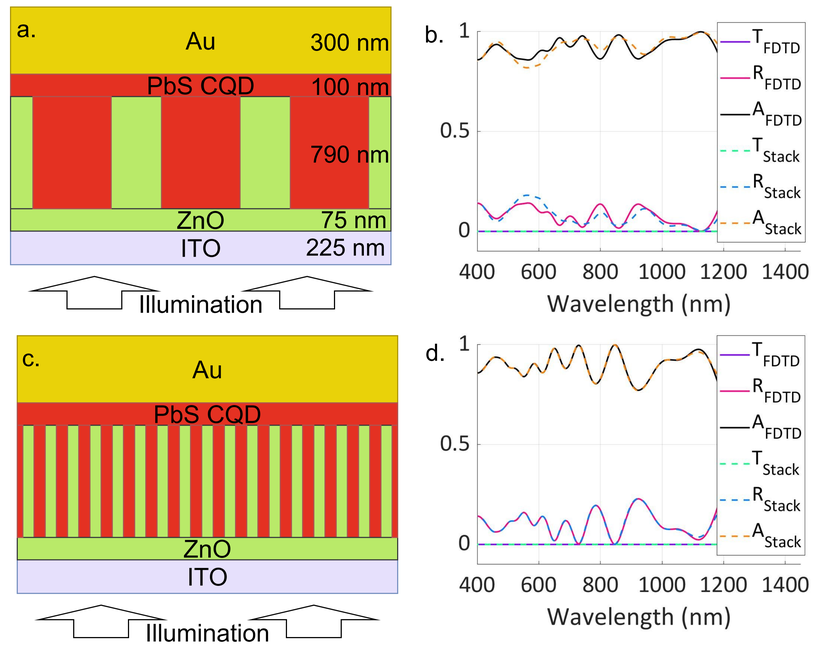

Figure 3: Comparison of the optical behavior of the solar cell. (a) depicts a solar cell simulated with an equivalent model and (b) the corresponding FDTD results compared to the optical stack solver, (c) contains the solar cell with an effective model was used and (d) contains the optical behavior comparison.

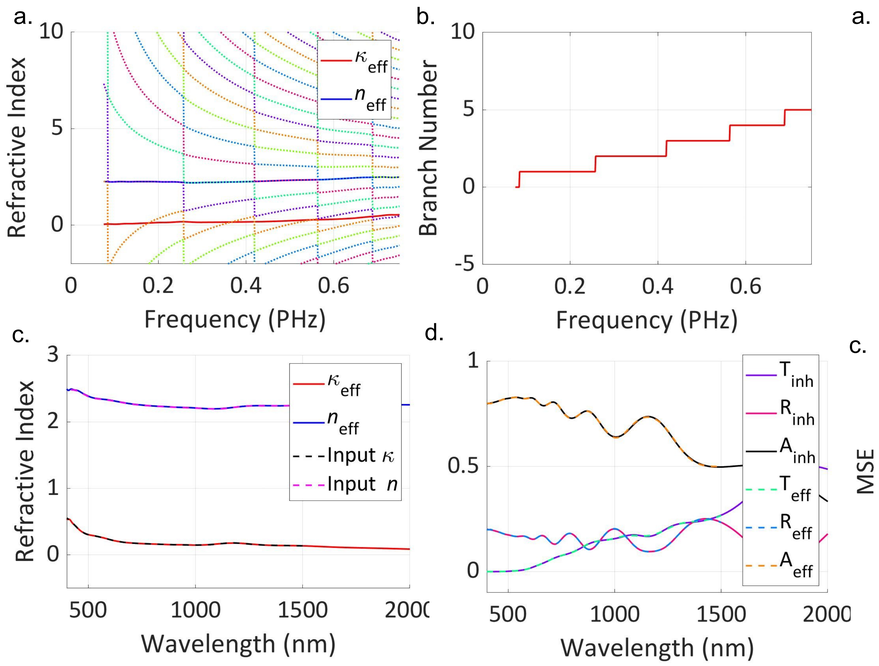

Figure 1: The method applied to a homogeneous slab of PbS CQDs. (a) Branches of the complex logarithm with the real and imaginary parts of the refractive index; (b) branch number as a function of frequency; (c) extracted refractive index compared to the known refractive index of the PbS CQDs; (d) optical behavior from FDTD compared to the method of this work.

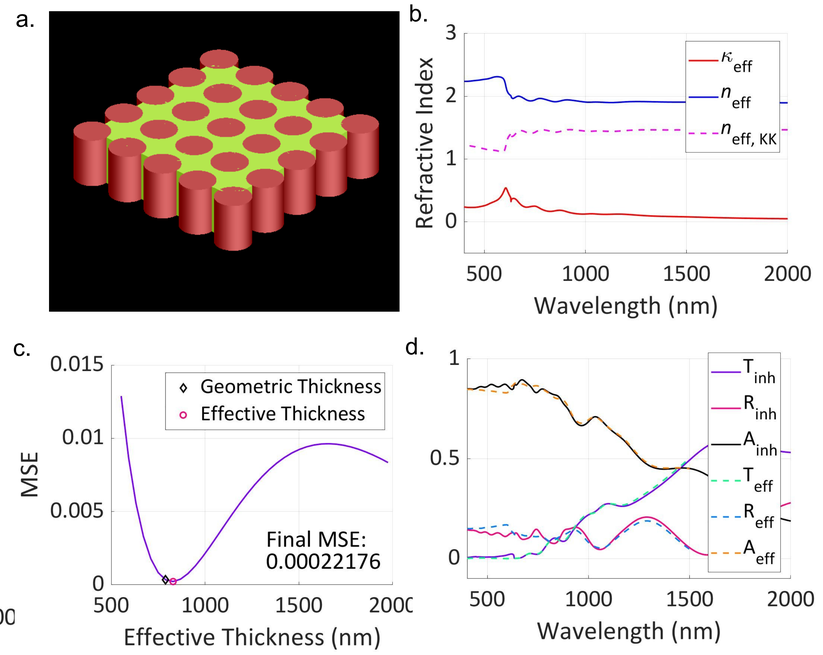

Figure 2: Homogenizing a patterned slab of PbS CQD nanodisks in ZnO. (a) The inhomogeneous structure with PbS CQDs (red) and ZnO (green); (b) the equivalent refractive index model with Kramers-Kronig relations; (c) MSE as a function of d_{eff}; (d) comparison of the optical spectra.

Solar Cell Simulation

We simulate the behavior of a PbS CQD solar cell, modifying the design in [1]. We replace the patterned layer by the equivalent slab calculated previously and simulate the solar cell using a fast optical stack solver. We also compare (Fig. 3) with a solar cell corresponding to an effective material model (feature size reduced by factor of 10).

Conclusions

We have introduced a simple and robust solution to the branching problem in the NRW method. Our method uses the lowest absolute mean derivative at low frequencies and enforces continuity, and then compares optical behavior to determine an effective thickness. We compare the method across effective and equivalent regimes. We demonstrate the fast and accurate simulation of a solar cell with our method and compare the regimes present there as well.

Additional Questions?

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References

[1] T. Kim, X. Jin, J. H. Song, S. Jeong, and T. Park, *ACS Energy Letters*, vol. 5, pp. 248–251, 2020.

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