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Surrogate based modeling and optimization of plasmonic thin film organic solar cells

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In this study, we demonstrate that surrogate models can be trained and used to accurately predict the optical properties of thin film solar cells and to optimize their structures. We consider organic an active thin film poly(3-hexylthiophene):(6,6)-phenyl-C61-butyric-acid-methyl ester (P3HT:PCBM) layer coated by indium-free highly conductivepolymer poly (3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS) on top with aluminum as cathode, and study optical absorptivity enhancement of such a structure when embedded with periodic spherical silver nano-particles. Metallic nano-structures, including textures, gratings and particles are known to induce plasmonic effects on the surface and inside absorbing semiconductors, thereby increasing light trapping in thin film cells. However, design of such structures requires precise characterization of the dependencies of electromagnetic field distribution to geometry parameters and material choices. Optical properties of structures at sub-wavelength scales are measured by numerically solving first principle electromagnetic equations, e.g., by means of finite difference time domain (FDTD) method. These methods are time-consuming, and therefore limit the possibility of exhaustive optimization. Surrogate modeling can be used to overcome this challenge. In the present work, we design a two-layer neural network (NN) surrogate model to estimate the optical absorptivity of the cell for any given geometry vector as well as any radiation wavelength and incident angle. Training of the network is done using the Levenberg–Marquardt (LM) method with generalization techniques such as early stopping and Bayesian regularization using a pool of training and validation data. The resulting surrogate model is first demonstrated to yield accurate out-of-sample estimation of absorptivity. Then, the model is used to investigate the individual contributions of each input by means of sensitivity analysis. In addition, optimization of the parameters is efficiently done using the surrogate model for different source light irradiance spectra and incident angles. Resulting optimizations are very efficient. At the end, solutions found by surrogate-based optimization demonstrate enhancement factors greater than 270% for optical absorptivity.

1. Introduction

Research on organic solar cells (OSC) has a two decade history with first mature examples studied and presented in 1990s [1,2]. Interest in these devices has led to record energy conversion efficiency of 11.5% as of 2015 [3], which is still significantly lower than achievable limits using silicon-based solar cells. Although power conversion efficiency of OSCs is lower than their inorganic counterparts, they provide other desirable characteristics such as low cost, ease of manufacturing and mechanical flexibility [4,5], as well as smaller diffusion length of primary excitons which allows comparably thinner active layers [6]. On the other hand, all photovoltaic devices suffer from losing optical thickness as the physical thickness of the active layer decreases [7,8]. Implementing metallic (plasmonic) nano-textures can help to improve optical absorptivity of thin film layers, therefore enhancing photocurrent by means of scattering and near field light concentration [9]. However, in order to properly design and fabricate such structures, a comprehensive understanding of the underlying electromagnetic interactions with plasmonic, dielectric and semiconductor mediums and interfaces at nano-scale is required. Gaining physical insight into dependency of optical performance of a thin film with shapes, dimensions, material choices and other parameters of plasmonic nano-textures or nano-particles have been the subject of extensive review by nano-technology experimental and computational scientists in the past 15 years. The research has led us to several

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Nomenclature

A	absorptivity
C	cost function
c_1, c_2	simulated annealing parameters
D	derivative vector
$\boldsymbol{e}$	error
EF	enhancement factor
g	probability
I	solar spectrum
J	Jacobian
L	number of layers
m, t	trend line parameters
N	number of data in sampled set
n_v	number of parameters in coefficient vector
$\mathbf{p}$	NN input
$\mathbf{q}$	re-normalized NN output
r	Ag radius
R	number of neurons
R_0	number of inputs
s	vertical distance of Ag from bottom
$\boldsymbol{s}, \boldsymbol{S}$	sensitivity
SSE	normalized mean sum of squared error
SSW	sum of squared weight
t	target output
T	temperature parameter in simulated annealing
t_1	P3HT:PCBM thickness
t_2	PEDOT:PSS thickness
$\boldsymbol{v}$	coefficient vector
W	coefficient matrix
$\mathbf{x}$	geometry vector
y_0, y_1, y_2	normalized NN input, intermediate output and output

Greek letters

α, β	regularization parameter
λ	wavelength
μ	Marquardt parameter
φ_1, φ_2	Lagrange multipliers
θ	incidence angle

Subscripts

b	bare
D	derivative
j	index of inputs
m	index of layer
p	plasmonic
T	training
V	validation

Superscripts

k	iteration
L	lower limit
n	index of data in sample set
U	upper limit

design guidelines. In general, it is agreed that particle shape, dimension and position in the solar cell should be taken into account for a rigorous design of a plasmonic solar cell [7]. In addition, precise computational simulators that model electromagnetic equations and material properties at nano-scale and solar optical wavelenghts should be accompanied by powerful optimization algorithms for a feasible and efficient design [10–15].

Optimal design of OSCs via plasmonic nano-material modifications has been recently focused by several researchers. In [16,17], a systematic study using Finite Element Method (FEM) was conducted in order to maximize absorption enhancement of a PEDOT:PSS/P3HT:PCBM/Al solar cell with Ag nanospheres embedded in P3HT:PCBM. It is demonstrated that an OSC with 33 nm active layer and 24 nm diameter Ag nanospheres can absorb as much light as a 61 nm active layer alone can. In [18], the authors used brute search method to improve solar cell efficiency using an optoelectrical simulation for ITO/PEDOT:PSS/P3HT:PCBM/Al with square Al grating. They achieved 17% improvement in efficiency compared to the bare solar cell. In [19], OSCs consisting of the layers Ag/MoO_3/P3HT:PCBM/Ca/ITO were optimized to maximize power conversion efficiency (PCE). 85 nm active layer and 5 nm MoO_3 was demonstrated to result in a PCE of 3.86%. However, in those studies, only one or two parameters were considered to be optimized; a complete optimization has never been done for the overall solar cell geometry.

Optical modeling of thin film solar cells relies on first principle calculations. Finite difference time domain (FDTD) and Finite Element Method (FEM) are two effective and common methods for solving Maxwell's equations. However, these computational methods require extensive resources and time. In a design optimization cycle where one is looking for the best set of nano-materials shapes and dimensions, many repeated numerical FDTD simulations must be carried out for an entire wavelength range. This makes the search process extremely cumbersome and, in cases with more than a handful of parameters, infeasible. Even state-of-the art numerical optimization algorithms might not be able to cope with such complexity at higher dimensions or in cases where time varying or non-stationary elements are present (e.g., when the light source changes or additional constraints are added and many optimizations need to be implemented). In lieu of further advances in first principle simulators, the only remedy to such a challenge is the use of "surrogate modeling". That essentially means replacing the black-box (FDTD simulations) by an accurate regression model which is able to "learn" the system's response by being "trained" with the previously generated data. Such a model can be used for both optimization and analysis, leading to the concept of Surrogate-Based Analysis and Optimization (SBAO). In addition to expediting the design of optimal parameters, SBAO can be used for a variety of analytical purposes, such as "Sensitivity Analysis", where the relative contribution of each input parameter to the output is quantified.

Surrogate modeling can be constructed by a variety of approaches, such as Kriging (KRG) model, polynomial regression (Response Surface Approximation (RSA)), neural networks or multi-layer perceptrons (MLP), and Gaussian radial basis functions (RBF)) [20]. It is worth mentioning that the use of SBAO in optimization of engineering systems is not unpresented. In fact, several recent work have addressed using RSA for optimization of micro-scale thermal systems (see e.g. [21]), obtaining a computationally-reduced electromagnetic simulations for transformers and antennas [22], and for designing high-performance buildings [23]. Such modeling however has never been applied to thin film solar cells and electromagnetic (FDTD) simulations of semiconductors and plasmonic structures to the best of our knowledge. The present work can therefore serve as an example use case of SBAO in thin film solar cell design and analysis, and shall moti-