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Application of artificial neural network for accelerated optimization of ultra thin organic solar cells

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ABSTRACT

In this study, we show that design optimization of solar cells can be accelerated using neural networks (NN) effectively. We consider an organic thin film solar cell consisting of a poly(3-hexylthiophene):(6,6)-phenyl-C61-butyric-acid-methyl ester (P3HT:PCBM) absorber, an antireflective indium tin oxide (ITO) layer and an aluminum back reflector layer. Zinc oxide (ZnO) and molybdenum trioxide (MoO_3) interlayers are also used as electron and hole transfer layers. Silver nanotextures are embedded within absorber layer to create near field effects thus enhancing optical absorption. 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 and finite element methods. 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 NN surrogate model to estimate the optical absorptivity of the cell for any given geometry vector as well as any radiation wavelength. After the preliminary optimization which utilizes NN, the result of optimization is obtained within narrowed optimization bounds obtained from the results of surrogate based optimization. A 325% of enhancement in absorption is obtained as a result of optimization.

1. Introduction

Organic solar cells (OSC) have attracted considerable attention as promising third generation photovoltaic devices due to ease of fabrication, inexpensive power generation and mechanical flexibility (Ameri et al., 2009; Gunes et al., 2007; Krebs, 2009) . However, power conversion efficiency of OSCs could only reach up to 11.5% as of 2015 ("Best Research-Cell Efficiencies," n.d.), which is significantly lower than inorganic counterparts. One of the methods to improve the efficiency is optical absorptivity enhancement by light trapping techniques (Atwater and Polman, 2010; Ferry et al., 2010; N'Konou et al., 2017). Light can be trapped inside the absorber layer of the solar cell by using an antireflective coating, metal back reflector and nanotexturing. The first option reduces the reflection while the rest creates near field effects and multiple scattering. Absorption enhancement in solar cells via plasmonic nanotextures has been the subject of extensive review in the nanotechnology field in the last decade (Enrichi et al., 2018). The research has led us to several design guidelines. In general, the size, shape and location of metallic nanostructures play important roles in absorption enhancement (Atwater and Polman, 2010; N'Konou et al., 2017), and poor designs can cause even decreased absorption (Shen et al., 2009; Vedraine et al., 2011; Zhu et al., 2014). Furthermore, optical modeling of solar cells at nanoscale should be accompanied by powerful algorithms for a complete design optimization (Hajimirza et al., 2012; Hajimirza and Howell, 2012, 2015, 2013a, 2013b).

Optical modeling of thin film solar cells requires solving Maxwell's electromagnetic equations which are a set of partial derivative equations of electric, magnetic and displacement fields. Except for a limited number of circumstances, Maxwell's equations are solved using computational tools, such as Finite Difference Time Domain (FDTD), Finite Element Method (FEM) and Fourier Modal Method (FMM). These tools are computationally expensive, thus they are more suitable to be used in the parametric studies where only a few parameters are optimized, rather than a simulation-based optimization of a full set of design variables.

Simulation-based optimization problems are not limited to the present study, and address a wide range of engineering fields (Golovin et al., 2017). Some examples are computational fluid dynamics (CFD) analysis, structural analysis (FEM) and electromagnetic simulations (FDTD, FEM,…), etc. The common practice to perform these simulations is utilization of commercial software packages which are conceptually a black-box taking input vector and returning a set of desired outputs. Surrogate-based optimization methods are developed for reducing computational cost of simulation-based optimization problems.

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These methods engage powerful optimization algorithms with the approximate alternatives for the high fidelity functions (Nguyen et al., 2014; Queipo et al., 2005; Rios and Sahinidis, 2013). There are various surrogate modeling techniques, such as polynomial regression, Gaussian process and neural networks. Among these methods, neural networks (NN) have the ability of approximating almost every function regardless of the degree of nonlinearity (Hagan et al., 2014). In recent years, NN has been very popular in solving engineering related problems such as geographic information systems (Pijanowski et al., 2014), meteorology (Jang et al., 2004), groundwater management (Dash et al., 2010), predicting physical properties of nanofluids (Heidari et al., 2016) and more. However, these models, and more broadly any particular surrogate modeling has never been used to model absorptivity of a solar cell based on its geometry for optimization.

Optimal design of plasmonic OSC devices has recently been studied by several researchers. Shen et al. (2009) conducted a systematic study to maximize absorption enhancement of a PEDOT:PSS/P3HT:PCBM/Al solar cell where Ag nanospheres are embedded inside the absorber layer. The authors studied the influence of the particle diameter and the distance between the particles on the absorption enhancement. Vedraine et al. (2011) also performed a detailed parametric study of the effect of Ag nanospheres on the optical absorption and obtained absorption enhancement factors up to 3. Fallahpour et al. (2015) conducted an optimization study based on a coupled optical-electrical analysis. A 17% of improvement was obtained in power conversion efficiency as a result of optimization. However, in all these studies, only a few design variables were optimized, and a complete OSC optimization is lacking. Furthermore, the hybrid optimization methodology used in this paper has never been used before to the best of our knowledge.

The rest of the paper is organized as follows: The physical model of OSC is presented in the next section. The details of the mathematical methods are given in Section 3 and the results are presented and discussed in Section 4.

2. Physical model

In general, a solar cell consists of an absorber, an antireflective coating and a back metal contact. It is also very common to use electron and hole transport layers (ETL and HTL). ZnO is mostly used as ETL due to its favorable optoelectronic properties (Beek et al., 2004, 2005; Ullah et al., 2017) and MoO_3 is a stable hole selective contact with nontoxic nature (Stubhan et al., 2015). The schematics of the solar cell structure used in the present study are shown in Fig. 1. In this design, the widely used organic bulk heterojunction blend P3HT:PCBM is preferred in the absorber layer, aluminum is selected as the cathode due to its low work function (Notarianni et al., 2014) and OSC is coated with anti-reflective indium tin oxide (ITO). Electron and hole transport layers, ZnO and MoO_3 are also included in the design to be optimized (Ou et al., 2016; Ullah et al., 2017).

Generally, optical efficiency enhancement of the solar cells is accomplished by improving radiation absorption. One way to improve absorption is to increase the physical thickness of the solar cell. However, that results in increased probability of recombination when the absorber thickness is larger than the collection length, therefore defying the original purpose of solar to electricity conversion of the cell. One way to enhance the optical performance without causing recombination is utilization of plasmon polaritons by metallic nanostructures. For this purpose, Ag nanostructures are embedded in the absorber layer. The nanostructures are located near MoO_3 because the absorption enhancement in a solar cell is shown in the literature (see e.g., Vedraine et al., 2011) to be larger when plasmonic nanostructures are placed away from the interface where light enters (back zone). Ag nanotextures have elliptical shapes. A 2D surface texture is aimed to be modeled with two diameters for the elliptical nano-textures. However, the same design can easily be extended to 3D by only adding more input variables, namely ellipsoid diameter and spacing variables in the z direction. Distance between nanostructures and ZnO layer is taken as a design variable instead of the overall thickness of P3HT:PCBM, in order to avoid a possible short-circuit. The improvement due to the presence of silver nanostructures can be quantified by absorption enhancement factor (EF). This is defined as the ratio of the number of photons absorbed by the absorber layer when the nanostructures are embedded, to the number photons absorbed by the bare solar cell. Namely:

$$EF = \left[\int \lambda \alpha_p(\lambda) I(\lambda) d\lambda\right]\left[\int \lambda \alpha_b(\lambda) I(\lambda) d\lambda\right]^{-1}, \quad (1)$$

where α_j is the portion of absorbed power when unit power light is propagated through the solar cell where $j = p$ for the plasmonic and $j = b$ for the bare solar cell. $I(\lambda)$ is the AM1.5 standard solar spectrum ("American Society for Testing and Materials, 2003, 'ASTM Standard Tables for Reference Solar Spectral Irradiances,'" n.d.). The integration is over the entire wavelength range of solar spectrum. In this study, the bare solar cell consists of aluminum, P3HT:PCBM and ITO layers and glass substrate (see Fig. 1).

The optimal size and configuration of silver nanostructures and the optimal layer thicknesses are sought in order to maximize EF. As underlined in the previous section, the absorbed power inside thin film solar cells can be calculated by solving Maxwell's equations. FDTD is one of the computational methods for solving Maxwell's equations on a discrete spatial and temporal grid called Yee's cells. For the present study, we have used FDTD Solutions software provided by Lumerical Inc. ("Lumerical Inc.," n.d.). Automatic mesh option of the software is used (mesh accuracy: 5, provided by software). Additionally, the mesh on the nanostructure is overwritten with a mesh size of 0.4 nm as a result of an extensive mesh independence study (not included here for the sake of brevity). The time step used in the simulations is 0.53×10^{-4} fs.

The material properties used in FDTD simulations are taken from literature (Hajimirza and Howell, 2014; Oueslati and Messaoud, 2015; Palik, 1998; Rand et al., 2004; Shen et al., 2009; Vos et al., 2016) and presented in Fig. 2.

3. Neural network based optimization

3.1. Neural network model of optical absorption

NN consists of artificial neurons which map the input space to the output space by means of coefficients and transfer functions in various layers. There may be multiple neurons in each layer, but the number of neurons in the first and last layers must equal to the number of input and outputs, respectively. NN has the capability of approximating almost every function regardless of the degree of nonlinearity (Foresee and Hagan, 1997; Hagan et al., 2014). NN represents the relationship between input and output as a series of functions evaluated at the artificial neurons. The output of the NN model is

$$\mathbf{y_i} = \mathbf{f_i}(\mathbf{W_i y_{i-1}}) \ , \ \forall \ \mathbf{1} \leqslant \mathbf{i} \leqslant \mathbf{L}, \mathbf{y_0} = [\bar{\mathbf{t}}_1, \bar{\mathbf{t}}_2, \bar{\mathbf{t}}_3, \bar{\mathbf{t}}_4, \bar{\mathbf{t}}_5, \bar{\mathbf{d}}_1, \bar{\mathbf{d}}_2, \bar{\mathbf{s}}, \bar{\lambda}, \mathbf{1}]^{\mathbf{T}} \quad (2)$$

where $\mathbf{y_i}$ is the normalized output vector and W_i is the coefficient matrix of the ith layer, and L is the number of layers. $\mathbf{y_0}$ is the input vector normalized to within the $[-1\ 1]$ range through the transformation . The output is then renormalized to $[0\ 1]$ to obtain NN absorptivity, $\alpha_{NN} = f_{NN}(\mathbf{x}, \lambda)$, where $\mathrm{x} = [t_1, t_2, t_3, t_4, t_5, d_1, d_2, s, 1]^T$. The last term of the input vector is 1 due to bias term in coefficient matrix. W_i is found as a result of NN training by minimizing the training cost function, $C(\mathbf{v})$:

$$C(\mathbf{v}) = \beta SSE + \alpha SSW \quad (3)$$

where $SSE = \mathbf{e^T e}$ is the sum of squared error between NN output and target and $SSW = \mathbf{v^T v}$ is the Bayesian regularization term where $\mathbf{v}$ is the vector concatenation version of coefficient matrices. SSW is a penalty term to avoid large coefficients which results in overfitting. α and β are regularization parameters set iteratively.

NN training is done using Levenberg-Marquardt (LM) method with