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Novel design of plasmonic and dielectric antireflection coatings to enhance the efficiency of perovskite solar cells

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ABSTRACT

Recently, nanostructured plasmonic antireflection coatings emerge as a solution to minimize reflection in solar cells over a wideband. However, metals have large light absorption coefficient, making this solution non-reliable for efficient large-scale production. On the other hand, all dielectric antireflection coatings are considered as promising alternative due to the lower losses and easier assembly, especially for third generation photovoltaics such as perovskite solar cells. Herein, we report a first principles methodology for selecting and comparing optimally nanostructured antireflective coatings for enhancing the efficiency of perovskite solar cells based on Mie theory. The first part of the method includes studying absorption and scattering cross sections of five nanostructures and identifying the role of magnetic and electric dipoles. Accordingly, dimensions of each nanostructure that maximizes light coupling to the solar cell active layer was identified. The second part comprises the study of the coupling effect between closed nanostructures. Using three-dimensional finite element method optical and electrical model, periodicity and dimensions of the proposed nanostructures with the highest generated photocurrent were identified. The results showed 15% enhancement in short circuit current (J_{sc}) over the entire wavelength band, and up to 27% in narrow band spectrum compared to planar perovskite solar cells.

1. Introduction

Perovskite thin film solar cells (TFSCs) have recently attracted the attention of the scientific community due to their unique optical and electrical properties, low fabrication cost, high carrier collection efficiency, and large-scale assembly (Yang et al., 2015; Fei et al., 2017). There are many limitations in Perovskite TFSCs performance, such as long-term stability and low light absorption percentage in the perovskite thin film layer. Stability issues are more related to the electrical properties of the materials. A recent paper suggests the use of reduced graphene oxide layer between gold back contact and hole transport material to enhance the stability of perovskite solar cells with +1000 h of stable operation time (Arora et al., 2017). However, the other drawback of perovskite TFSCs is their lower light absorption within the active layer due to the small active layer thickness. In this regard, light trapping nanostructures inside active layer (Xiao et al., 2018; Bawendi and Hess, 2018; Abdelraouf and Allam, 2016; Wu, 2018), or metal nanoparticles (Islam et al., 2014; Islam et al., 2015; Abdelraouf et al., 2017) were used to enhance the optical light absorption in many types of solar cells. Recent techniques for enhancing the efficiency of perovskite TFSCs, in particular, are based on the concept of using antireflective coating using silica nanospheres (Luo et al., 2018; Zeng et al., 2017), or nanophotonics to design front nanoarchitectures (Paetzold et al., 2015), or light trapping nanostructures inside the active layer (Abdelraouf and Allam, 2016), or plasmonic nanostructures atop the metal back contact (Adhyaksa et al., 2017).

Recently, plasmonic nanostructures have been integrated in many optoelectronic devices due to their various advantages, including the possibility to guide electromagnetic waves at a dielectric/metal interface using surface plasmon guided modes (SPGM) (Schmidt and Russell, 2008), control the direction of light scattering using subwavelength metallic nanostructures, high suppression of reflected light in the wavelength range of the nanostructure resonance, confine light at subwavelength scale due to large localized surface plasmon resonance (LSPR) (Atwater and Polman, 2010), possibility of tuning light reflection from substrate by changing particles dimensions, shape, interparticle distances, or material. Despite all these advantages, plasmonic nanostructures have some serious limitations. For instance, most of the used metals have large imaginary refractive index in the optical wavelength range, leading to large light losses (Johnson and Christy, 1972) or the formation of Schottky barrier at the dielectric/metal interface that may reduce collection efficiency of charge carriers in solar

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cells (Zhou et al., 2014). To this end, plasmonic nanostructured materials have been explored as antireflection coatings to improve the efficiency of TFSCs, due to their capability to control the far field light scattering directivity from nanoparticles front active layer, confine near field light in the subwavelength scale for nanoparticles rear active layer, and increase the short circuit current and photoconversion efficiency (Gu et al., 2012). For instance, the use of nanostructured silver front in a-Si:H TFSCs fabricated by nanoimprinting lithography shows enhancement in the power conversion efficiency from 6.32% to 9.6% (Ferry et al., 2011). Also, P3HT:PCBM-based solar cells showed an increase in the short circuit current by 2.7 mA/cm^2 upon the use of silver nanoparticles front active layer (Morfa et al., 2008). The same organic material showed an enhancement in the photoconversion efficiency from 3% to 3.65% upon the deposition of gold nanoparticles front active layer (Lee et al., 2009).

Currently, dielectric nanostructures emerged as promising alternatives to plasmonic nanostructures (Spinelli et al., 2012; Raman et al., 2011; Ren and Zhong, 2018). Most of the used dielectrics are semi or fully transparent in the optical wavelength range, resulting in negligible light losses inside the dielectric nanostructures. Also, the high refractive index of the used dielectrics enables the control over light directivity at the nanoscale via tuning the magnetic and electric Mie resonance of the nanostructures. Solving Mie theory (Bohren and Huffman, 2008) for small sphere in free space analytically using spherical harmonic enables the calculation of electric and magnetic multi-poles of the sphere versus the wavelength. Note that Mie resonance refers to peaks of these electric or magnetic multi-poles (Zhao et al., 2009). Tuning the absorption Mie resonance could change the light reflection minima wavelength. Also, changing scattering Mie resonance enables the coupling of incident light into the waveguide modes of the substrate. In this regard, titanium dioxide (TiO_2) is one of the most widely used materials for different solar cells due to its large refractive index ($n \approx 2.7$), low optical losses in the visible and near-infrared wavelength ranges (Yang et al., 2016), and possibility of tuning its Mie resonance via changing the dimensions and the shape of the nanostructures. Moreover, all-dielectric antireflection nanostructured coatings have been emerged as promising alternatives to overcome the disadvantages of plasmonic nanostructures while having the ability to control the incident light at the nanoscale for many nanophotonics applications (Krasnok et al., 2015). Changing the dimensions of silicon nanopillar-based structure enables wideband antireflection for photovoltaic systems (Bezares et al., 2013). Many research works showed promising results of integrating dielectric nanostructures in solar cells, such as depositing silicon dioxide SiO_2 nanospheres over a-Si:H TFSCs that enhanced the photocurrent by 15% compared to flat a-Si:H TFSCs (Grandidier et al., 2011). Also, introducing gallium phosphide (GaP) nanoscatterers on top of the active layer of a-Si:H TFSCs improved the photoconversion efficiency from 8.1% to 9.89% (Wang and Su, 2014). Experimental realization of dielectric nanostructures for enhancing generated photocurrent have been already reported in literature using back contact nanostructures (van Lare et al., 2015) and front dielectric nanostructures (Tamang et al., 2016).

Herein, we demonstrate a fast estimation method for selection of silver nanostructured coatings to control the direction of the scattered light from perovskite solar cell substrate. The performance is also compared to that of the low optical losses and high index dielectric TiO_2 coating. Our method is based on two separate approaches: (1) Mie scattering theory to investigate the role of optical resonance (electric or magnetic) in the proposed subwavelength nanostructures and its role on enabling guided resonance modes in the underlying perovskite active layer (Brongersma et al., 2014) and selection of the dimension of each studied nanostructure that achieve the highest light coupling in the substrate. (2) investigating the role of coupling between closed optimally dimensions of the nanoscatterers on a substrate. Through the optical model, we examined the role of periodicity on the overall guided light resonance modes inside the substrate. After selecting dimension and periodicity for each studied plasmonic and dielectric antireflection nanostructured coatings, we used the electrical model to calculate the power conversion efficiency of the promising designs. The main advantage of our proposed method is that it can be applied for any solar cell substrate and enables the design of antireflection coatings that are very close to the exact solution.

2. Modeling details

Two separate three-dimensional (3D) electromagnetic wave (EMW) models, based on finite elements method (FEM) COMSOL multi-physics software, were used to construct the model. The first part of the model was built based on the concept of Mie scattering theory to calculate the normalized absorption cross-section (NACS) and normalized scattering cross-section (NSCS) of the proposed scatterers. The second part was based on coupled optical-electrical model to simulate perovskite solar cells with suggested optimally top scatter nanostructures to calculate the overall efficiency of the solar cells. For simulating NACS and NSCS for scatterers on a substrate, we used full field EMW to calculate the incident electric field profile on planar substrate only. Then, we couple this electric field profile as a background field in scatter field EMW for a nanostructure on a substrate. These steps were mandatory because the optical properties of a particle on a planar dielectric surface differ dramatically from those of the same particle embedded in homogenous medium (Lermé et al., 2013). Incident plane waves in full field EMW consider both s-polarization and p-polarization with normal incidence in the z-direction, and use the AM1.5G solar spectrum as an input power in the range of 300–800 nm with a step of 10 nm. The simulation was performed on cell volume surrounded with perfect matched layer (PML) in all directions, and periodic boundary conditions (PBCs) in x-y direction were considered. A tetrahedral mesh type was used with a size below one-tenth of the lowest simulated wavelength in the simulated cell size. Furthermore, a mapped mesh was used in the PML layer to reduce the overall mesh number. The NACS of the studied nanostructures was calculated using Eq. (1):

$$NACS = \frac{W_{abs}}{P_{inc} * Surface \quad Area} \tag{1}$$

where W_{abs} is the amount of absorbed power in the nanostructure [W], which is calculated by integrating the resistive energy loss over the volume of the nanostructure, P_{inc} is the energy flux of the incident wave [W/m^2]. The NSCS was calculated using Eq. (2):

$$NSCS = \frac{W_{sca}}{P_{inc} * Surface \quad Area} \tag{2}$$

where W_{sca} is the scattered energy rate [W]. Scattered energy rate came from integrated scattered energy over the surface surrounding the nanostructure. P_{inc} is the energy flux of incident wave [W/m^2]. For comparison and selection of optimally nanostructures on a substrate, we defined a parameter called active area absorption enhancement (AAAE), which represents the enhancement in the coupled power to the substrate after depositing the nanostructure on top of the surface. AAAE is the ratio between the integrated power absorbed in the substrate in the presence of a scatterer to the integrated power absorbed in case of a planar substrate only, Eq. (3).

$$AAAE = \frac{\iiint |E|^2_{scatter \quad on \quad substrate} \; dVd\lambda}{\iiint |E|^2_{planar \quad substrate} \; dVd\lambda} \tag{3}$$

Upon the dimensions selection of each nanostructure with the highest AAAE, we simulated the coupled optical-electrical model to calculate the efficiency of the solar cells. The optical model used the same setup of the EMW model in the first part. The active layer absorption was calculated using Eq. (4):

$$Absorption \quad (\lambda) = \frac{|E_{active \quad area} \quad (\lambda)|^2}{|E_{Total} \quad (\lambda)|^2} \tag{4}$$