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Revisited design optimization of metallic gratings for plasmonic light-trapping enhancement in thin organic solar cells

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ABSTRACT

We revisit previous studies of metallic gratings for optical absorption enhancement in an organic solar cell with a thin active layer. Our device geometry is designed for a real solar cell with full of functional layers. Various metallic gratings calibrated to generate periodic scatterers and low reflectors for broadband light account for increases in short circuit current density of up to 47% when compared to its flat counterpart. We found that the tapered grating has greater performance than the regular rectangular grating for transverse magnetic (TM) polarization while the latter shows better performance for transverse electric (TE) polarization. The overall metallic grating induced absorption enhancement was found at all angles of incidence. The best configuration was realized for the tapered grating-based solar cell at 25° of inclination.

1. Introduction

Photovoltaic (PV) research is attempting to low-cost and high-manufacturability solar cells. Thin-film organic solar cell (OSC) is a promising candidate for such a route because of its cheaper production and higher manufacturing volume [1]. The primary obstacle to reach this route is the low efficiency of current OSCs. Significant improvement in the cell efficiency is required to make them competitive with grid power [2]. One of the most challenges in achieving higher efficiencies is absorbing enough light in the thin active layer and the short diffusion length of carriers. OSCs' thicknesses are restricted by physical limitation due to the need to utilize electrical characteristics of the material. If the active layer becomes too thick, it will cause significant reduction in exciton collection from recombination within the active layer [3,4]. Absorbed photons propagate through the active layer before enough may be converted to excitons, because of the thickness restraint. In addition, too thick active layer beyond carrier diffusion length will result in current loss due to recombination. Thus, the tradeoff between enough absorption and minimizing recombination is the key challenge in designing OSCs.

Recently, the utility of metallic nanostructures within various forms such as nanoparticles, nanogratings, and nanocavities in solar cells has been demonstrated to provide optical field enhancement, and improvement of the optical absorption [5–12]. This plasmonic light-trapping is able to absorb sunlight over a moderately broad bandwidth of operation owing to the excitation of tunable plasmonic modes in these metallic nanostructures.

Properly placing metallic nanostructures inside the active layer can strongly enhance absorption via near-field enhancement effects [5]. However, near-field absorbed sunlight may not contribute in the generation of photocurrent due to the metal losses and the induced quenching effect of the excited states at the metal/active layer interface [13]. Isolating the plasmonic nanostructures with an inert coating can reduce the electric losses, but decreases the near-field absorption. These detrimental effects are among the reasons why plasmonic light-trapping results in the limited improvement of the photocurrent generation in OSCs as reported in literatures [14,15]. The same scenarios happen with plasmonic gratings designed at the OSC's back reflector which is theoretically predicted to improve the light absorption [16], but experimentally reported on the less power conversion efficiency [17]. The absorbed light did not contribute to the generation of photocurrent and dissipated inside the metal heating up the electrode.

Alternative ways to enable the light-trapping enhancement associated with the photocurrent generation improvement is to put the metallic nanoparticles/nanogratings on top of the cells [18–20]. These plasmonic nanostructures can act as periodic optical antennas for light and store energy in the localized surface plasmon resonance (LSPR). On the other hand, combined plasmonic gratings on the top and bottom of the polymer active layer

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can complementary enhance optical absorption [21]. However, this two-layer cell consisting of a polymer active layer and a metal back reflector is impractical since the basic simplest form of the OSC structure should consist at least three layers made by sandwiching a layer of organic electric material between two metallic conductors. These two metallic layers have different work function to generate strong electric field in the organic layer. When the light is absorbed in the organic layer, electrons will be excited to the lowest unoccupied molecular orbital and leaves holes in the highest occupied molecular orbital, thereby generating excitons. The induced potential from the different work functions assists to split the exciton pairs, pulling electrons to the positive electrode and holes to the negative electrode [22]. In this letter, we theoretically investigate metallic grating influence on the absorption efficiency and the short circuit current density of real OSCs consisting of functional layers as practical devices. We consider various shapes of metallic gratings including rectangle and taper. More specifically, we optimize these gratings put on the active layer of the practical OSC to enhance the optical absorption. We found that the tapered gratings could provide more absorption enhancement than rectangular gratings thanks to their ability to induce near-field enhancement and less reflection.

2. Solar cell structure and modeling method

A schematic of the practical OSC investigated is shown in Fig. 1. The transparent anode is made by 100-nm-thick indium tin oxide (ITO) and deposited on a 20-nm-thick highly conductive hole transport layer, poly (3, 4-ethylenedioxythiophene): poly (styrenesulfonate) (PEDOT). The polymer active layer consists of the electron donor poly(3-hexylthiophene) (P3HT) and the electron acceptor (6,6)-phenyl-C61-butyric-acidmethyl ester (PCBM) with 1:1 weight ratio in contact with the cathode made of silver (Ag). Silver is chosen since it has low metal absorption loss and has benefits of the excitation of surface plasmon resonance modes suitable for enhancing a P3HT: PCBM OSC. The active layer's thickness in all investigated OSCs in this work is chosen to be 50 nm since it can support the Fabry–Perot resonant mode in a planar cell structure without gratings, which is able to resonantly trapping incident sunlight. Combing with other plasmonic modes associated with metallic gratings, we expect to absorb light over a broad bandwidth of operation using this 50-nm thin film. Apart from the possibility to excite Fabry–Perot mode to resonantly absorb sunlight, the 50-nm-thick active layer benefits PV's research attempts to realize thinner solar cells than current practical PCBM: P3HT OPV, which is about 200–250 nm for their low-cost and higher-volume manufactory.

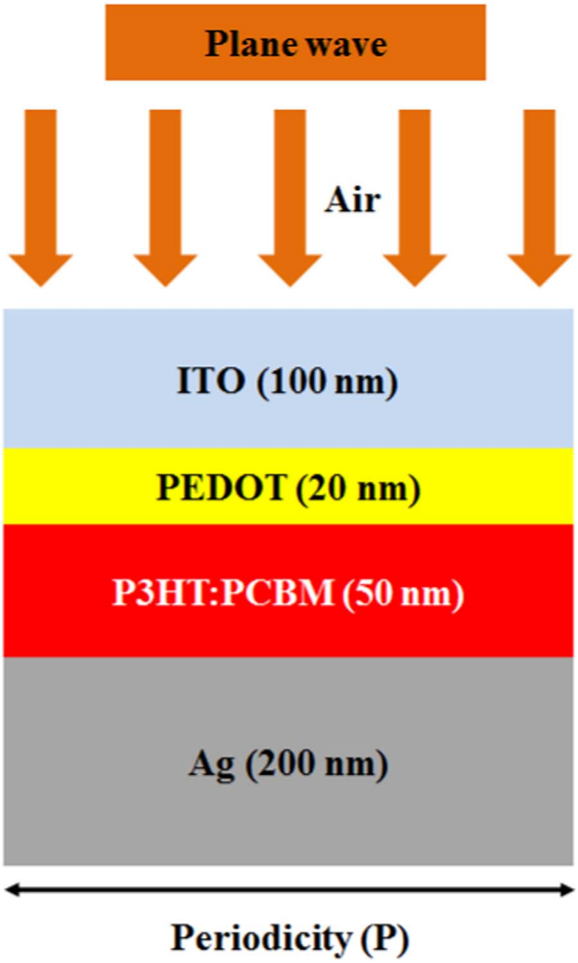

Fig. 1. Cross-section of the reference flat OSC.

There exists several numerical techniques that have been successfully employed to calculate the light absorption of the active layer of solar cells, including finite-difference time-domain (FDTD) methods, finite-element methods (FEM), the transfer matrix model (TMM) and the rigorous coupled wave analysis (RCWA). In this work, the calculation of light absorption is performed by the FEM-based COMSOL package [23]. Owing to the periodic nature of the OSC structure, only one unit cell with a lattice constant of P is needed for calculations of the whole structure. We assume the sunlight illumination on the cell as incident plane waves having wavelengths of 300–800 nm which is the region of interest for the P3HT: PCBM material. Proper periodic boundary conditions are set at the left and right boundaries, while perfectly matched layer (PML) absorbing boundary conditions are used at the top and bottom boundaries of the computation domain. The absorption (A (λ)) in the active layer is calculated by integrating the divergence of the Poynting vector ($\vec{S}$, power flow) which is then normalized with input power P_0 as follows:

$$A(\lambda) = \frac{\int(\nabla\cdot\vec{S})dA_{active\ \ layer}}{P_0},$$

where $A_{\text{active layer}}$ is area of the active layer.

The short circuit current density (J_{SC}) is subsequently calculated based on the absorption as in [10].

3. Result and discussion

3.1. Enhanced absorption by silver rectangular gratings

The metallic gratings integrated on top of the solar cell (on top of the contacts) have been demonstrated to be able to provide optical field enhancement, resulting in larger optical absorption. On the other hand, putting gratings on top of solar cell can result in high scattering of light and trap light effectively in the active over a broad bandwidth [21]. However, such a solar cell is impractical since it missed a conductive top contact to make a different work function to generate excitons. Using the gratings on the real device with additional layers of ITO and PEDOT may influence on their plasmonic effects. In this work, we propose to integrate plasmonic gratings in the PEDOT layer of the practical OSC. We investigate and optimize the gratings to get maximum achievable photocurrent density, so called short circuit current density.

The sketch of the proposed rectangular grating (RG)-based device structure is shown in Fig. 2. This configuration is expected