Optical Materials 84 (2018) 158–165

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Polarization-tuned chromatic electrodes using hybrid design of graphene-aluminum nanocross arrays for efficient organic solar cells

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ARTICLE INFO

Keywords:
Active color filters
Chromatic electrodes
Graphene
Aluminum
Energy harvesting
Organic solar cells

ABSTRACT

Solar cells entailing multi-coloring capability can pave the way for solar-powered colorful displays. Therefore, the energy that is usually wasted in color displays could be harvested to produce useful electrical power. On the other hand, introduction of color filters with capability of active control on the output color results in more compact and efficient optical devices. In this work, we have proposed a chromatic electrode in which the transmitted light has been employed as a source for the solar energy device while the reflected light generates polarization-tuned colors, simultaneously. Aiming to design such a chromatic electrode, a hybrid nanostructure of graphene and aluminum nanocross arrays has been employed for the first time. In addition to replacing ITO in organic solar cells by a novel electrode and achieving performance enhancement of organic solar cells, mapping the polarization of the incident light to visible color results in solar-powered chromatic polarizers with potential applications including active color displays, security tags, and polarization imaging. Using finite-difference time-domain numerical simulations, it has been shown that the proposed nanostructured electrode leads to enhanced photocurrent densities in the range of 11.82–17.05 (mA/cm^2) due to the light trapping plasmonic properties of the nanocross arrays. Additionally, replacing ITO, suffering from poor mechanical properties and cost-ineffectiveness, offers a promising approach for large-area growth of organic photovoltaics.

1. Introduction

Photovoltaic devices with multi-coloring functionality can open the way for solar-powered colorful displays as a new approach for future energy harvesting devices [1–5]. Among photovoltaic technologies, organic solar cells (OSCs) have become really attractive due to their outstanding features, such as light weight, cost-effectiveness, semi-transparent properties, and flexibility [6]. However, the trade-off between the thickness of active layer to maximize the solar absorption and the charge recombination is a challenge while designing OSCs [6]. Accordingly, utilization of light manipulating techniques plays a crucial role in performance enhancement of organic photovoltaic (OPV) devices [7].

Engineering the light behavior to minimize the reflectance has been a key method to enhance the efficiency of solar cells. Meanwhile, it has been demonstrated that controlling optical characteristics can be possible by employing various nanostructures and nanoparticles which can even offer wavelength selectivity (especially advantageous for sensing and color filtering applications [1,8–17]). Therefore, one promising approach for improving the solar performance has been utilization of nanoparticles [18–22], plasmonic nanostructures [23–30], and diverse anti-reflective coatings (ARCs) [31–39].

Indium tin oxide has been known as the common transparent electrode in most OSCs [40–43]. Unfortunately, ITO is not suitable for large-scale production due to the limited reserves of indium [44]. Moreover, the low escalating conductivity of ITO on flexible substrates and its poor mechanical properties make this material inappropriate for flexible devices [45]. Thus, it would be greatly advantageous to utilize various transparent electrodes [46–48] to replace ITO in OSCs. Among the reported transparent electrodes, periodic 2D nanostructures (which are polarization insensitive under the normal incidence of light) have attracted great deal of attention since they can yield flexible and cost-effective ITO-free OSCs. For instance, plasmonic nanohole arrays have already been designed as transparent electrodes in ITO-free OPVs while utilizing their field enhancements to improve the solar absorption [45,49,50]. Nevertheless, utilization of alternative transparent electrodes to replace ITO, especially for development of highly efficient OSCs, has not widely been studied yet [45].

Graphene is an ideal alternative to ITO due to its outstanding features, such as high transparency, conductivity, high electron and hole carrier mobility, and thermal and mechanical stability as well as offering a large surface area. These features make this material a good

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https://doi.org/10.1016/j.optmat.2018.06.044
Received 25 April 2018; Received in revised form 16 June 2018; Accepted 19 June 2018

candidate for OPVs [51]. Accordingly, in some previous studies, graphene films have been proposed as transparent conductive electrodes in OSCs [52–60]. Further improvement of these graphene-based OPVs and utilization of hybrid design of graphene-nanostructures are still under investigation [24,61].

On the other hand, color filters have recently become important components in display technologies. Achieving new approaches to realize active coloring operation like in polarization-tuned plasmonic filters [62,63] have also become really attractive for diverse interesting applications including polarization imaging, polarimetry, and controllable and invisible tags. However, considerable amount of light energy is usually wasted in optical displays. Therefore, methods that harvest the wasted energy can lead to self-powered energy-efficient displays [1].

In this paper, a hybrid structure based on graphene and aluminum nanocross arrays has been proposed aiming to realize polarization-tuned chromatic electrodes for the first time. In addition to replacing ITO with an efficient nanostructured electrode, the designed OSC yields broadband performance enhancement and improved photocurrent densities thanks to the light trapping properties of the plasmonic Al nanocross arrays. Using numerical simulations based on the finite-difference time-domain (FDTD) method, enhanced photocurrent densities of about 11.82–17.05 (mA/cm^2) have been achieved. Moreover, tuning the polarization angle offers an active color filtering operation, simultaneously. This dual functionality is a promising approach for self-powered active color displays and light harvesting devices. In contrast to conventional color filters which can realize a single color, our proposed structure results in dynamic colors by controlling the polarization of the incident light. This feature also makes the designed solar-powered structure appropriate for many interesting applications, such as polarization microscopy and polarimetry. The proposed chromatic electrode also benefits from aluminum-based plasmonic advantages, such as great tunabilty, CMOS-compatibility, stability to manufacturing procedures, and low cost.

This paper is organized as follows: after introducing the proposed device and its detailed design procedure in section 2, the simulated optical characteristics of the designed structure have been investigated in section 3. Finally, a summary of the work has been presented in section 4.

2. Design method

A schematic and cross section view of the proposed chromatic electrode is depicted in Fig. 1(a). As seen, the nanostructure entails a hybrid design of graphene and Al nanocross arrays. In fact, in a typical fabrication process, after chemical vapor deposition of graphene on a polished quartz substrate [64], Al nanocross array of 40 nm thickness can be generated using electron beam lithography [62]. The reason to use the nanocross arrays is that the horizontal and vertical arms of a cross shape are polarization sensitive, so the optical responses of the device would not be the same for different polarization states resulting in active control on the output color of the filter [62]. Additionally, the plasmonic properties of the proposed nanocross array can lead to light trapping thus performance enhancement of the designed OSC. Utilizing Al for this design is advantageous owing to the outstanding features of this material, such as its low-cost and abundance, CMOS-compatibility, and its amenability to the fabrication procedures [65–68]. Meanwhile, Al demonstrates great optical properties as a promising material for plasmonic color filters thanks to its strong and broadly tunable plasmon resonances with its interband transition located outside the visible and near-ultraviolet wavelength spectra [67]. In addition, since the aluminum's plasma frequency is higher than that of gold or silver, and it is placed in the ultraviolet region, the absorption of Al is relatively slight in the visible range [65,69]. Therefore, Al offers a good candidate for realization of transparent electrodes [69,70], and it has been predicted theoretically that the optical and electrical performances of Al meshes should outperform other metals, such as gold, silver, copper, and nickel [71]. Accordingly, Al has been the best choice for our chromatic electrode design. The large semi-transparent graphene film, entailing the advantages mentioned in the previous section, makes this material a good candidate for the design of a transparent electrode. Meanwhile, employing the nanocross array results in polarization-tuned dynamic coloring operation as well as light harvesting properties. The low reflectance of the proposed nanostructure and its light trapping properties lead to broadband performance enhancement of the OSC and improved photocurrent densities. The entire designed OSC is also demonstrated in Fig. 1(b). As shown, the proposed nanostructured electrode can be placed on top of the whole OSC aiming to replace ITO as the top electrode.

Generally, the OSC can be deposited on a quartz substrate with millimeter-order thickness. For the optical simulation of this work, employing a micrometer-order substrate is sufficient in order to simulate the solar cell behavior accurately. Here, the structural parameters of the nanocross arrays have been designed based on the previously reported chromatic polarizer [62] owing to its appropriate polarization-tuned properties (see Table 1). It has to be noted that the array pitch (period) refers to the distance between the centers of two adjacent crosses as shown in Fig. 1(a).

For design of the OPV solar cell, a 190 nm film of the well-known bulk hetero-junction blend of poly-3-hexylthiophene P3HT and [6,6]-phenylC61-butyric acid methyl ester PCBM (P3HT:PCBM) has been employed aiming to realize the photoactive layer. Moreover, a 50 nm film of poly (3,4-ethylenedioxythiophene)-poly (styrenesulfonate) (PEDOT:PSS) has also been employed as the hole transporting layer [72]. To realize the back electrode, a 500 nm Al layer has been utilized.

In order to investigate the optical properties of the proposed solar cell, FDTD simulations have been employed. A schematic of the simulation setup can be observed in Fig. 2. Aiming to model the solar light, a normal incident plane-wave source has been used. For reducing the simulation time, just one periodic unit-cell with perfectly matched layers (PMLs) boundary conditions (BCs) along z direction has been simulated. The polarization angle of the source (the angle ϕ shown in Fig. 1(b)) has been set in the model analysis group. For the transverse magnetic (TM) polarized light (when the polarization angle is 0°, so the electric field is oriented in the x direction), the group will automatically use anti-symmetric and symmetric BCs along x and y axes, respectively aiming to reduce the simulation time. For the transverse electric (TE) polarized light (when the polarization angle is 90°, and the electric field is oriented in the y direction), the symmetric and anti-symmetric BCs along x and y axes, respectively will be employed. Additionally, a non-uniform mesh refinement has also been exploited to ensure the simulation accuracy. To obtain the optical characteristics for different polarization angles, two simulations are necessary. In fact, the optical properties of an arbitrary linear polarization have been achieved by summing the results from TM and TE polarizations with appropriate weighting [62]. Such simulations have been performed by running parameter sweeps. Different monitors have been utilized to simulate the required optical characteristics of the device. For instance, to calculate the absorption in the active layer (P3HT:PCBM), two power monitors have been used as shown in Fig. 2.

3. Results

The effect of tuning the polarization angle (the angle ϕ shown in Fig. 1(b)) on the resultant transmission and reflection spectra of the proposed nanostructured electrode applied to the designed OSC is depicted in Fig. 3(a) and Fig. 3(c). As the horizontal and vertical arms of a cross shape are polarization sensitive, the optical responses of the device are not the same for different polarization states. As seen, transmission dip (reflection peak) varies between 560 and 410 nm while the polarization angle changes from 0° to 90° in 10° steps. Additionally, the functionality of the proposed design as a semi-transparent electrode can