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Performance improvement of ultrathin organic solar cells utilizing light-trapping aluminum-titanium nitride nanosquare arrays

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ABSTRACT

Despite the crucial role of plasmonic nanostructures in enhancing the performance of organic solar cells, the actual absorption of the active layer in these cells is restricted by the parasitic metal absorption loss limiting their efficiencies. In this paper, a bilayer of Al-TiN nanosquare array has been proposed as a novel plasmonic scheme in order to improve the photocurrent and the solar absorption of organic solar cells. The hybrid design of Al and TiN materials reduces the parasitic loss issue offering extended application of plasmonic light-harvesting structures. Engineering the energy band diagram of the cell and concentrating the electrical field distribution inside the active layer result in boosting the absorption as well as the optical current densities for each layer. Utilization of TiN in the proposed design also benefits from the cost effectiveness, abundance, and CMOS compatibility of this material compared to noble metals as well as featuring appropriate light trapping properties. In addition, the symmetric scheme of the proposed structure makes it polarization insensitive under the normal incidence. The numerical simulations of this study based on the finite-difference time-domain (FDTD) method show an enhanced absorption of 70–88% over the spectral range of 300–625 nm and the maximum enhancement factor of 2.16 at the wavelength of about 665 nm. Moreover, an improved photocurrent density of 13.7082 (mA/cm^2) has also been achieved despite the usage of an ultrathin active layer. The proposed design can also be developed to achieve performance enhancement of other thin film solar cells in the future.

1. Introduction

Solar energy has attracted great deal of attention as a clean, inexhaustible and environmentally friendly source of power offering an excellent alternative to fossil fuels. In spite of the significant research advances on photovoltaic cells in recent decades, their large-area usage has still been limited due to the high cost [1]. Employing thin film photovoltaic cells has been interesting since they can be made in flexible substrates and reduce the amount of material resulting in cost-effective approaches [2,3]. Using thin film technology can also reduce the recombination rate causing a rise in open circuit voltage (V_{oc}) (especially when the criterion of light confinement is met) [4,5]. Among the well-known thin film photovoltaic systems, organic solar cells (OSCs) have become really interesting thanks to their cost-effectiveness, simple manufacturing process, and compatibility with diverse flexible substrates [6,7]. However, due to the low charge carrier mobility of the active layer, it is required to reduce the recombination losses in organic photovoltaic cells [8]. Therefore, an important challenge with these cells is the trade-off between increasing the thickness of the photoactive layer and decreasing the recombination loss [9].

Increasing the solar absorption by controlling the light behavior has been a key method to boost the efficiency of the solar cells. Meanwhile, it has been indicated that engineering the optical properties can be achieved by utilization of various plasmonic nanoparticles and nanostructures which can even lead to selective characteristics like in sensing and color filtering applications [10–20]. Hence, such plasmonic schemes can also be applied leading to impressive enhancement in performance of thin film solar cells [21–32].

Such plasmonic enhancement methods have recently been employed aiming to improve the performance of OSCs [33–35]. This improvement originates from their surface plasmon resonances and the consequent near-field concentration yielding light trapping properties [36]. In fact, the matching between the frequency of incident light with that of collective oscillation of electrons leads to formation of localized surface plasmon resonances (LSPRs) [37].

For instance, plasmonic based OSCs using gold (Au) and silver (Ag) nanoparticles have previously been proposed owing to their low ohmic losses [38–41]. Despite the outstanding plasmonic properties of Au and Ag in the solar spectrum region, these metals suffer from high cost, incompatibility with conventional industrial technologies, and low

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temperature and oxidation stability [42].

Aluminum (Al)-based plasmonics offers higher plasma frequency overcoming the absorption loss in blue and ultraviolet wavelengths which can broaden the scattering enhancement range [43]. Moreover, this material offers strong and tunable plasmon resonances making it suitable for light manipulating applications [44,45]. However, the plasmonic loss of Al is not negligible especially in the wavelength regions where the absorption of common active materials needs to be improved [46]. As a result, broadband enhancement of photoactive layer absorption is still a challenge while designing thin film solar cells. For example, a study on the bi-layer design of Al and Ag nanogratings have previously been proposed [47].

Recently, novel plasmonic materials, such as transition metal nitrides specifically titanium nitride (TiN) have become greatly attractive. This is mainly because of the unique features of this material ranging from its cost-effectiveness, low loss, temperature and oxidation stability, and CMOS compatibility unlike Au and Ag [48–51] as well as offering characteristics similar to the behavior of metals [52,53]. Hence, some previous studies have been reported introducing TiN-based plasmonic schemes for feasible applications in the visible and infrared spectral regions [53–57]. TiN nanoparticles have also been employed in order to enhance the performance of silicon and organic solar cells, lately [37,48,54,58]. It has been demonstrated that TiN and Au nanoparticles show similar behaviors while TiN also benefits from the mentioned advantages, simultaneously [37].

In this paper, we have proposed a nanosquare array of TiN-Al bilayer aiming to utilize their light trapping properties for performance enhancement of OSCs. For this purpose, FDTD numerical simulations have been employed in order to improve the solar absorption and enhance the photocurrent density. Despite the usage of an ultrathin photoactive layer, the simulation results indicate an enhanced absorption and photocurrent density (J_{sc}) of 13.7082 (mA/cm2). Using TiN in the proposed design can extend the potential application of plasmonic light-trapping techniques. This paper is organized as follows: after introducing the proposed scheme and its detailed design method in section 2, the optical simulation results of the structure have been investigated in section 3. Finally, a conclusion of the work has been presented in section 4.

2. Design method

A schematic and 2D cross section of the designed structure is shown in Fig. 1. As seen, nanosquare arrays of single layer (of 60 nm-thick Al film) and bilayer (consisting of Al and TiN films with thicknesses of 40 nm and 20 nm, respectively) incorporated with organic cells have been employed (see Fig. 1(a) and (b)). In order to design these plasmonic nanostructures, Al and TiN have been utilized so that light trapping and performance enhancement of the proposed cell can be realized, simultaneously. The symmetric geometry and square shape of the nanoparticles results in polarization insensitive behavior of the design under normal incidence. This feature makes the device appropriate for practical applications where it is required to deal with unpolarized light.

The applied material to realize the active layer is the commonly used bulk hetero-junction blend of poly-3-hexylthiophene P3HT and (6,6)-phenylC61-butyric acid methyl ester PCBM (P3HT:PCBM) with 1:1 wt ratio [59]. This 50 nm ultrathin film functions as a combination of donor (P3HT) and acceptor (PCBM) materials. For the transparent conductive electrode, a 10 nm-thick film of highly conductive polymer, poly 3, 4-ethylenedioxythiophene: polystyrenesulfonate (PEDOT:PSS) with the work function of 5ev [1] has been exploited. Therefore, the designed OSC is indium tin oxide (ITO)-free, so it benefits from cost-effectiveness, good flexibility, temperature and chemical stability [41,60]. For the back electrode, a 100 nm Al layer has been used. Material properties have been extracted from literature [61–63]. The energy level diagram of the proposed cell is shown in Fig. 2. When the light hits the structure from the top side, absorption of the input photons results in the generation of excitons (bound electron-hole pairs). These excitons then diffuse to the acceptor/donor interface. After that, the generated excitons can dissociate leading to the formation of free-charge carriers owing to the energy difference between electron affinity of the acceptor and donor.

FDTD numerical simulations have been employed to calculate the optical properties of the proposed structure. A summary of the applied simulation setup is depicted in the 2D cross section of Fig. 3. To simulate the light source, a transverse magnetic (TM) polarized normally incident plane wave has been utilized hitting the structure from the top side (see Fig. 3). (Despite the usage of a TM polarized source due to the polarization insensitivity of the designed structure, the effect of polarization has also been tested by simulating the unpolarized light). To reduce the simulation time, a unit-cell with periodic BCs along x and y axes (antisymmetric BCs along x axis and symmetric BCs along y axis) and perfectly matched layers (PMLs) have been used. A non-uniform mesh refinement has been utilized to achieve more simulation accuracy. The required optical properties have been extracted by utilization of appropriate monitors.

The optimal structural parameters (the width (W) and period (P) shown in Fig. 1) of the Al-TiN nanosquares have been calculated using a numerical method based on the absorption enhancement. As will be discussed in section 3, the optimum values of W and P are 140 nm and

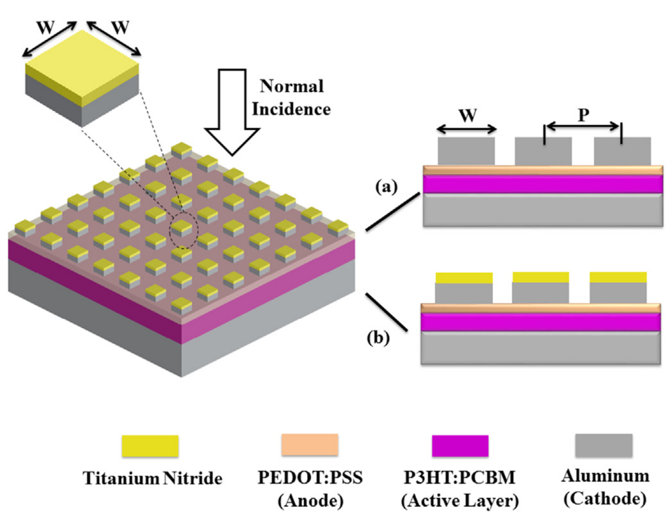

Fig. 1. A schematic and 2D cross section of the proposed OSC incorporated with (a) single layer and (b) bilayer of Al and TiN nanosquare arrays.

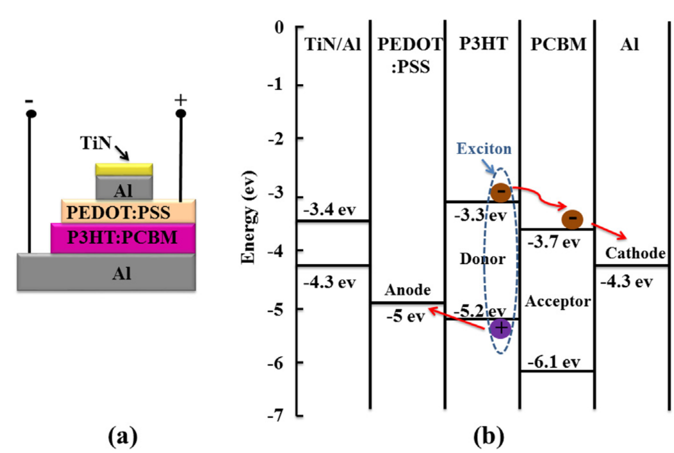

Fig. 2. (a) The cross section view and (b) band energy diagram of the proposed cell.