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Tailoring of the plasmonic and waveguide effect in bulk-heterojunction photovoltaic devices with ordered, nanopatterned structures

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A B S T R A C T

Various nano-patterned bulk-heterojunction (BHJ) films with different diameters and pitches were fabricated by a stamping method to tailor the plasmonic effect. The nanopatterned BHJ active layers exhibit regular-ordered embossing structures, which were confirmed by the surface morphological analysis with SEM and AFM. The simulation results confirm that devices with nanopatterned BHJ film with a diameter/pitch of 265/400 nm exhibit a strong improvement in E-field distribution intensity due to the combination of the plasmonic and waveguide modes compared to devices without a nanopattern, with 150/400 nm, or with 265/800 nm, which led to increased J_{SC} and cell efficiency in J–V curves under solar light illumination. The optimized plasmonic effect plays an important role in the light harvesting of BHJ devices.

1. Introduction

Bulk-heterojunction (BHJ) solar cells with a conjugated polymer donor and fullerene derivative acceptor have received considerable interest and been developed over decades due to their promising advantages of large-area mass production on flexible substrates through a low cost, simple solution process [1–7]. The power conversion efficiency (PCE) of the organic solar cell is determined by three parameters, including the open circuit voltage (V_{OC}), fill factor (*FF*), and short circuit current (J_{SC}). The V_{OC} is related to the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor [8,9]. The *FF* is affected by the BHJ film nanomorphology and device series resistances (R_s) [10,11]. The J_{SC} is determined by the absorption spectrum of the composed materials of the BHJ and the photo-generated charge carriers from the BHJ film with nanoscale morphology [12–14]. To enhance the PCE of the BHJ solar cells, the nanoscale phase was separated, but a three-dimensional interpenetrated donor–acceptor active film morphology within a very thin film thickness around 100 nm is an important factor for efficient exciton dissociation, charge separation, and collection [15–17] Recently, low band gap materials (polymer and small molecules), which have a large absorption spectrum [18–20], newly designed device structures (inverted structures and tandem cells) [21–23], detailed optimized processing conditions (annealing, additive, thickness, and interlayer) [24–26], and a plasmonic effect

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from nanopatterns and nanomaterials [27–30], have been broadly researched to improve the PCE in organic solar cells. As a result, the PCE of BHJ devices has reached a maximum of 9–10% with the potential for commercialization [19,22].

Typically, the optimum cell performance of most BHJ solar cells is observed in a very thin BHJ layer of approximately 100 nm because of the inherent poor charge transportation of organic materials. Therefore, not all of the incident photons can be fully absorbed by the thin active layer. As a possible solution to overcome this drawback, regular-ordered nanopatterned structures in the BHJ solar cell that induce improved light absorption and trapping in the limited thickness of the active layer, i.e., the plasmonic effect, have been considered. Recently, the plasmonic effect was demonstrated in BHJ polymer solar cells [31,32] and tandem solar cells [33,34] with a significantly increased PCE, primarily attributed to the enhanced light concentration and harvesting caused by the scattering and near-field excitation [35–38]. Improved light absorption of the BHJ leads to enhanced J_{SC} and PCE values of the devices. However, there are few reports on the systematic investigation of plasmonic effects from nanopatterns [35,39,40] on BHJ cell performances via finely controlled BHJ nanostructures. Here, we demonstrate tailoring of the E-field distribution intensity in BHJ solar cells with various sizes of two-dimensional dot (2D-dot) nanopatterns that induce improved light absorption and harvesting. BHJ solar cells with different, well-ordered hole patterns exhibit different enhancements of current density due to the tailored E-field distribution intensity, as was confirmed by FDTD simulation.

2. Experimental details

2.1. Preparation of PUA–PC Film with 2D-dot nanopatterns

Clean, silicon master molds with a diameter/pitch of 150/400, 200/400, 265/400, and 265/800 nm and a height of 50 nm were prepared and treated with trichloro-(1H,1H,2H,2H-perfluorooctyl)silane (FOTS) to reduce the surface energy. Self-assembled monolayers (SAMs) were then generated on the surface. The UV-curable resin: poly(urethane acrylate) (PUA) was dropped on top of the flexible polycarbonate (PC) film, and the film was flattened using a roller. Different sizes of nanopatterned PUA–PC film were successfully fabricated after curing with a 365 nm UV light and detaching the silicon master mold.

2.2. Fabrication of the BHJ photovoltaic devices

The ITO–glass substrate was prepared through a cleaning procedure using detergent, acetone, and isopropyl alcohol with the sonication process. The ITO was then treated by UV-ozone for 20 min, and the hole transporting layer

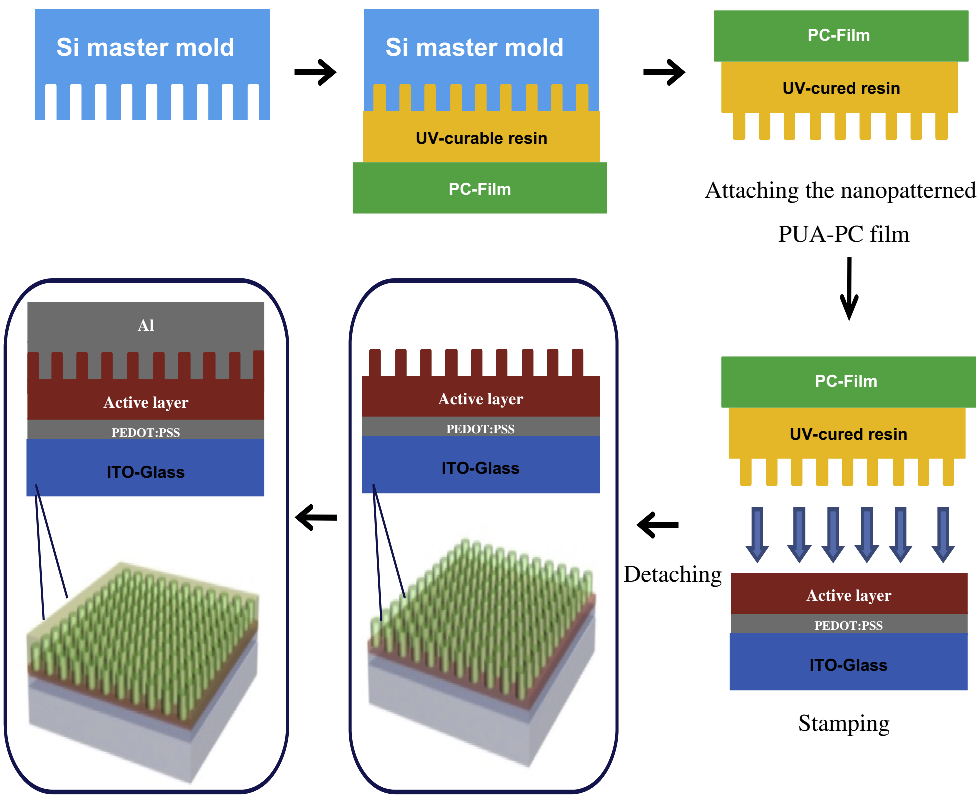

Fig. 1. Fabrication schematic diagram of the 2D-dot nanopatterned BHJ active layer with the help of a PUA–PC film replica film from a master mold by a stamping process, and their application in photovoltaic devices.