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Investigation of Polymer/Si Thin Film Tandem Solar Cell Using TCAD Numerical Simulation

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Abstract: The current study introduces a two-terminal (2T) thin-film tandem solar cell (TSC) comprised of a polymer-based top sub cell and a thin crystalline silicon (c-Si) bottom sub cell. The photoactive layer of the top sub cell is a blend of PDTBTBz-2F as a polymer donor and $PC_{71}BM$ as a fullerene acceptor. Initially, a calibration of the two sub cells is carried out against experimental studies, providing a power conversion efficiency (PCE) of 9.88% for the top sub cell and 14.26% for the bottom sub cell. Upon incorporating both sub cells in a polymer/Si TSC, the resulting cell shows a PCE of 20.45% and a short circuit current density (J_{sc}) of 13.40 mA/cm^2. Then, we optimize the tandem performance by controlling the valence band offset (VBO) of the polymer top cell. Furthermore, we investigate the impact of varying the top absorber defect density and the thicknesses of both absorber layers in an attempt to obtain the maximum obtainable PCE. After optimizing the tandem cell and at the designed current matching condition, the J_{sc} and PCE of the tandem cell are improved to 16.43 mA/cm^2 and 28.41%, respectively. Based on this TCAD simulation study, a tandem configuration established from an all thin-film model may be feasible for wearable electronics applications. All simulations utilize the Silvaco Atlas package where the cells are subjected to standard one Sun (AM1.5G, 1000 W/m^2) spectrum illumination.

Keywords: all-thin-film; polymer-based cell; c-Si; Tandem solar cell; VBO; current matching; TCAD simulation

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1. Introduction

Photovoltaics propose promising solutions to the energy demand issue. Various types of solar cells have been widely presented and published. The central goal of recent research is to achieve efficient solar cells with a low cost of fabrication [1–3]. The generations of solar cells can be summarized in four generations. First, a generation based on the crystalline-silicon (c-Si), and gallium arsenide. Second, a generation based on amorphous and microcrystalline thin film silicon, copper indium gallium selenide (CIGS), cadmium sulfide (CdS), and cadmium telluride (CdTe). New compounds like organics, polymers and perovskites, and structures like tandem solar cells (TSCs) are the base of the third generation [4–8]. According to the non-toxicity, stability, abundancy, and well-known technology of silicon, silicon solar cells demonstrate the highest share of solar cells' market. The power conversion efficiency (PCE) of silicon solar cells exceeds 26% [9]. Additionally, many efforts have been conducted in order to achieve low-cost silicon solar cells [10–14]. Recently, a generation based on the insertion of the stable inorganic generation into the flexible, and low-cost polymers like metal-nanoparticles, and metal-oxides has been developed.

Bulk heterojunction polymer solar cells are gaining attention as they have the potential to provide flexible, lightweight, and cost-effective alternatives to silicon-based solar cells [15]. Researchers have been working on improving the charge selectivity of inverted