Solar Energy Materials and Solar Cells 176 (2018) 288–294

Contents lists available at ScienceDirect

Solar Energy Materials and Solar Cells

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

A practical wave-optical hemispheroidal nanostructure strategy for photonic-enhanced thin film solar cells

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ARTICLE INFO

Keywords:
Photovoltaics
Nanophotonics
Light trapping
Thin film solar cells

ABSTRACT

The interaction between light and wavelength-sized photonic nanostructure is highly promising for light management applied to thin-film photovoltaics (PVs). In this work, we put forward a practical wave-optical dielectric hemispheroidal nanostructure strategy under cost-effective anodic oxidation approach and substrate transfer method. By adjusting the oxidation voltage, periodic hemispheroidal nanostructure with diametral scale over 650 nm was obtained. Due to their wavelength-scale dimension, enhanced diffraction behavior and guided resonance were identified through finite-difference-time-domain (FDTD) simulation resulting in significant forward-scattering capabilities. The coherent optical performance was investigated experimentally and theoretically. To leverage the benefits of hemispheroidal nanostructure, amorphous silicon absorb layer and solar cell were fabricated. Compared with the planer structure, the developed hemispheroidal nanostructure could significantly improve the absorption of a-Si:H layer via light management with a 10.97% enhancement in the overall external quantum efficiency. Effective improvements in Voc and FF performances were also obtained in comparison to an etched AZO structure with high surface roughness. As the first demonstration, it was found that the hemispheroidal nanostructure by coating on the surface of a-Si:H thin film solar cells led to 7.79% and 7.38% enhancements respectively in overall energy conversion efficiency in comparison to the planar and the etched AZO structure.

1. Introduction

Photovoltaic (PV) devices can directly convert solar energy into electricity and have received considerable interest worldwide as promising candidates for harvesting clean and renewable solar energy. In order to advance the widespread of PV technologies, material cost of solar cells need to be continuously decreased and energy conversion efficiencies need to be further increased. Therefore, advanced light-trapping concepts in solar cells are essential [1]. Due to the significantly reduced thickness, light trapping (i.e., increasing the path length of incoming light) plays a critical role in the performance of thin film silicon solar cells and modules incorporating amorphous (a-Si:H) or/and microcrystalline (μc-Si:H) silicon as the absorber materials [2–5]. The resultant optically thicker but physically thinner devices imply cheaper and faster fabrication and also improve flexibility that is important for their application in bendable substrates [6], aiming for consumer-oriented products, such as sun-powered intelligent packaging [7], wearable PV, and portable electronics.

The conventional light trapping approach is the insertion of rough and randomly textured surfaces at the rear or front of the solar cells to diffuse light and thus increase its optical path length within the absorber layer [8–10]. In the last decade, the research on nanophotonic light-trapping concepts for the construction of periodic nanostructures has experienced a vast development, including prototyping in thin-film solar cells made of silicon [11–14], organic materials [15,16], GaAs [17], and Cu(In,Ga)Se_2 [18]. Several light trapping effects come into play in the wave optics regime of such structures, which crucially depend upon the parameters of the photonic and absorbing elements. The most prominent strategy of employing a periodic nanostructure is to make use of diffractive coupling of incident light to leaky waveguide modes supported by the absorber layers of the solar cells, thereby enhancing the absorption of incident light in the wavelength range of low absorptance [12,14].

A number of light trapping schemes have been proposed and

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https://doi.org/10.1016/j.solmat.2017.08.037
Received 1 June 2017; Received in revised form 30 July 2017; Accepted 29 August 2017
Available online 21 November 2017
0927-0248/

demonstrated using nanostructures, such as nanopillars [19], nanowires [20,21], nanodents [22,23] and nanospikes [24]. Spheroidal and hemispheroidal nanostructures have been indicated to be preferable to those with corners or edges (e.g., typical texturing features, nanocones, nanocylinders and nanowires, etc.) for light management applied to thin film solar cells because sharp terminations produce strong localized near-fields, whose energy is generally dissipated as heat but not used for current generation [25]. Additionally, spheroidal geometries exhibit lower sensitivity to the angle of incidence of the illumination, which is critical to increasing the acceptance angle of non-tracking PV devices [13].

The current study aims to demonstrate a viable and convenient route towards low cost fabrication of hemispheroidal nanostructure for photonic-enhanced thin film solar cells. Since the nanoarray is incorporated onto the front cell surface, this material should have low imaginary part of the refractive index and negligible absorption in the spectral range of cell photocurrent. A lossless optical material, aluminum oxide, was therefore selected. Comparable dimensions to the illuminating wavelengths were obtained through an anodic oxidation and etching procedure. Hemispheroidal nanostructures were arranged in a single layer of a square lattice by a delicate operation. The incorporation of a highly transparent and conductive ITO layer was produced before a-Si:H deposition. A numerical mesh-based finite difference time domain (FDTD) formalism was employed to model the coupled optical and electrical field distribution produced in the nanostructures. Although a-Si:H was used as the model material in this work, the developed hemispheroidal nanostructure can also be used for other types of thin film PV devices, such as organic solar cells and emerging high performance perovskite solar cells.

2. Experimental methods

Transparent anodic aluminum oxide (AAO) arrays with hemispheroidal nanostructure were fabricated through a two-step anodization process. All of the electrochemical experiments were conducted in a two-electrode electrochemical cell using a graphite counter electrode and a potentiostat (Hua Tai electronics co., LTD, HCP10-250) equipped with a voltage multiplier. The electrolyte temperature was accurately controlled by a Julabo refrigerated/heating circulator (Ping Xuan scientific instrument co., LTD) and were validated using a glass thermometer before each experiment.

A highly conductive ITO front contact layer was included between the alumina nanostructure and the p window layer in the cell model for lateral carrier collection using RF magnetron sputtering from a ceramic In_2O_3:SnO_2 target (In_2O_3: 90 wt%, SnO_2: 10 wt%) in a KJLC Lab-18 sputtering system. The chamber was evacuated to 8×10^{-8} Torr before deposition. Processing pressure, substrate temperature, and power density were kept at 2 mTorr, 200 °C and 0.12 W/cm^2, respectively. A 120-nm thick ITO layer was obtained after 80 min deposition with sheet resistance R_{sq} around 30 Ωsq^{-1}. With the much smaller thickness of ITO layer compared with the lateral dimension of the nanostructure texture, we obtained the conformal hemispheroidal nanostructure for the ITO surface. As surface morphology is important for light management in thin film solar cells, the characteristics of conformal structures are beneficial to the optical and electric field simulations.

The deposition of the a-Si:H *p-i-n* cells was carried out by a lab-assembled multi-chamber cluster tool. Plasma enhanced chemical vapor deposition (PECVD) at a frequency of 13.56 MHz and temperature ~ 200 °C was applied for the solar cell deposition process. The intrinsic a-Si:H(i) layers were deposited using a SiH_4:H_2 mixture of 40:200 sccm at the base pressure of 10^{-8} Torr and the working pressure of 0.5 Torr. For doping of the *p*- and *n*-layers, B_2H_6 and PH_3 were added, respectively. The thickness of the *p/n*-type doped layer and intrinsic absorption *i*-layer was fixed to 10 nm, 25 nm and 200 nm, respectively, which represented a compromise between absorption and stability against light-induced degradation [26]. A 100 nm ZnO thin film was inserted between the n and the metal contact layer for protecting the n layer from silver diffusion. Finally, a silver back contact (thickness of 100 nm) was deposited on top of the device by thermal evaporation through a shadow mask in order to define the cell area of 0.253 cm^2.

Atom force microscope (AFM; SPA 800, SII Nanotechnology) was carried out to investigate surface morphology and cross-sectional feature of the hemispheroidal nanostructure. The scattering transmittance (T_{sca}) was evaluated using a UV–Vis–NIR spectrophotometer (Carry 5000, Varian) with an integrating sphere. Current-voltage (J-V) characteristics and spectral response were determined by using a Wacom solar simulator (WXS-156S-L2, AM1.5GMM) and a quantum efficiency system (QEX10, PV Measurement), respectively. The external quantum efficiency (EQE) curves of all the solar cells in this study were determined at 0 V biased voltage. From the measured J-V curves, the open-circuit voltage (V_{oc}) and fill factor (*FF*) were obtained and the current densities were normalized with the short-circuit current density (J_{sc}) values obtained from *EQE* measurement.

A 3D finite-difference time domain (FDTD) numerical method was employed to rigorously model the optical and electrical effects of wave-optical hemispheroidal nanostructures on the thin film solar cells [23,25]. The method solves Maxwell's equations in arbitrary geometries and materials, one of the preferential approaches to tackle electromagnetic problems in the wave-optics regime, particularly for PV light management due to its conceptual simplicity and versatility. It is a time-domain method that the solutions can cover a wide frequency range with a single simulation run [2,27]. The scattering fraction and electrical field intensity $|E|^2$ distribution were calculated for the hemispheroidal nanostructure achieved here. As a function of wavelength for each of the materials used in the simulation, the optical constants were measured in the laboratory by ellipsometry WVASE32 and then fitted to the FDTD data by a multi-coefficient model, which accurately accounts for broadband linear material dispersion [28].

3. Results and discussion

We first prepared the transparent AAO arrays with hemispheroidal nanostructure referring to the first step of a “two-step anodization” method. Briefly, a piece of pure aluminum foil was electropolished in a mixture of perchloric acid and ethanol (1:4, v/v) at 5 °C for 3 min to remove surface irregularity and any potential contamination. High purity (99.999% purity) aluminum foil with thickness of 0.1 mm was selected for peeling convenience. Anodization was then carried out using 0.1 M phosphoric acid at 140–180 V and 2 °C for 2 h. A long anodization is necessary to increase the surface regularity. The first anodization step forms an oxide layer on the surface and begins the development of random pores. Continued anodization greatly improves the regularity in pore arrangement, yielding a straight pore array and an ordered cell configuration. After the first anodization, we etched away the porous alumina layer by using an alumina etchant (1.8 wt% chromic acid and 6 wt% phosphoric acid) at 65 °C for 4 h, excavating an ordered concave pattern onto the surface of the aluminum specimen. A second anodization was then conducted for 30 min using the conditions identical to the first anodization in order to complete the synthesis of the aluminum oxide nanoarray. The rest of the aluminum substrate was then dissolved in a mixture of HCl and $CuCl_2$ solution, leading the aluminum oxide layer to periodically hemispheroidal nanostructure. The remaining AAO layer was then suspended in the solution. A lift-up method was implemented during the next transplantation approach. An eagle XG glass was vertically dipped under the AAO template and afterward very slowly withdrawn, followed by a steam removal approach in a low vacuum chamber at room temperature. Finally, the hemispheroidal nanostructures were transplanted onto the eagle XG glass surface. Fig. 1 illustrates the overall preparation and fabrication procedure. In order to enhance the adhesion, a glass substrate etching process in HCl and H_2SO_4 mixing solution was primarily performed before the peeling and transplanting processes. The AAO nanostructure