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Research paper

Anti-reflective structures for photovoltaics: Numerical and experimental design

Kuan W.A. Chee [a,c,*], Ziqiang Tang [b], Hong Lü [a,d], Feng Huang [c]

[a] Department of Electrical and Electronic Engineering, Faculty of Science and Engineering, University of Nottingham Ningbo China, Ningbo 315100, China
[b] Department of Electrical and Computer Engineering, Faculty of Applied Sciences, University of British Columbia, Vancouver, BC, Canada V6T 1Z4
[c] Key Laboratory of Marine Materials and Related Technologies, Zhejiang Key Laboratory of Marine Materials and Protective Technologies, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, China
[d] Yisci Bio Co. Ltd., 3377 Kangxin Gonglu, Pudong District, Shanghai, 200120, China

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ABSTRACT

The effects of different anti-reflective structures on the photovoltaic performance of the silicon solar cell were studied using finite-element modelling and numerical simulations for which experiment alone does not provide a full description. The front surface reflectivity may be mitigated significantly by an anti-reflective coating (ARC) of a suitable thickness. Alternatively, nanoscale surface texturing can effectively trap a greater ratio of incident light to increase optical absorption. The optimized layer thicknesses of the ZnO single layer and SiO_2/Si_3N_4 double layer films were calculated for minimum reflectivity, with the former grown by magnetron sputter deposition and characterized using specular X-ray reflectivity measurements. Based on geometric ray-tracing and solutions to the semiconductor equations, the theoretical photovoltaic performance was simulated and compared for a range of incident angles at an optical intensity of 0.1 Wcm^{-2}, revealing a limit to the angular collection efficiency of the ARC at a grazing incidence angle of 30°. Using ZnO or SiO_2/Si_3N_4 ARCs or surface texturing increases the power conversion efficiency by 20%, 24% and 30% respectively at normal incidence. The insights provided by physical-based modelling on the optimized design parameters of the anti-reflective structures confer a promising pathway for enhancing the external quantum efficiency of photovoltaic devices.

1. Introduction

Over the past decade, the real price of electricity around the world has largely risen significantly, eg. by 63% in the U.K. (OVO Energy, 2018) or at 3% each year in U.S.A. (EnergySage, 2017a, b), partly driven by energy shortages owing to reliance on fossil fuels. On the contrary, the price of crystalline silicon photovoltaic panels has plummeted dramatically from $ 74 per watt in the early-1970s to less than 70 ¢ per watt in 2014 (Brown et al., 2015), and continuing to exhibit trends consistent with Swanson's law to date. Besides, solar energy delivers environmental benefits; the Solar Energy Industries Association reported that current levels of solar photovoltaic installation in the U.S.A. offset 37 million metric tons of carbon emissions (equivalent to planting 956 million trees) each year (EcoWatch, 2016), and the U.S. Environmental Protection Agency avers that carbon emissions can be slashed by 3 to 4 tons annually per two-person household by installing a solar power system (EnergySage, 2017a, b). Therefore the perceived socio-economic and environmental impacts continue to inspire the long-standing interest in harnessing sunlight to generate clean and sustainable electricity, with photovoltaic devices based on crystalline silicon wafers being the dominant technology in the solar energy market.

However, the power conversion efficiency (PCE) of crystalline solar cells is generally limited by the reflection of light at the surface, charge recombination and trapping in the material, energy dissipation caused by the cell's resistance, and temperature (Chanta et al., 2015; Filipowski et al., 2017; Chen and Shao, 2011; Cuce et al., 2013; Chander et al., 2015a, b). For bare or polished silicon, a significant fraction of the optical losses is due to the high index contrast resulting in a high surface reflection of nearly 35% over the complete AM1.5G spectrum. An approach to enhance optical absorption is therefore to design the front surface with anti-reflective structures that reduce reflection losses and enable increased photogeneration in the cell. The majority of the world's commercial silicon photovoltaics have so far relied on using single layer TiO_2, Si_3N_4 or SiO_2, but we explore ZnO single layer

* Corresponding author at: Department of Electrical and Electronic Engineering, Faculty of Science and Engineering, University of Nottingham Ningbo China, Ningbo 315100, China.
E-mail address: kuan.chee@nottingham.edu.cn (K.W.A. Chee).

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anti-reflective coating (SLARC) and SiO_2/Si_3N_4 double layer anti-reflective coating (DLARC) and benchmark with surface texturing. An anti-reflective coating (ARC) of transparent conducting oxide or dielectric material such as ZnO or SiO_2/Si_3N_4 thin films, when fabricated on the surface with an appropriate refractive index and film thickness, not only increases the short circuit current density through optical absorption and photogeneration, but like the ITO on SiO_2 (Drabczyk et al., 2016) or SiN_x:H (Kluska and Panek, 2016) layers, can passivate recombination sites and increase the open circuit voltage and fill factor. Specifically, the ZnO thin film is non-toxic and versatile, having high radiation tolerance at high temperature, is transparent in the visible region (Godlewski et al., 2009), and its synthesis relates to an established industry standard fabrication process. As a result, ZnO ARCs show a lot of promise for adoption in new technology solar cells. Without an expensive thermal budget, an experimental SLARC of ZnO was grown to an optimized thickness by RF magnetron sputter deposition on the crystalline silicon solar cell, and the layer thickness was measured using a specular X-ray reflectivity (XRR) technique. The emergent SiO_2/Si_3N_4 double layer thin film is known for its broadband transmissivity, which bestows a high absorption rate at shorter wavelengths. Furthermore, crystalline silicon surface texturing at the micro-/nano-scale can be applied to increase light trapping. In this paper, the effectiveness of the aforementioned anti-reflective structures will be investigated and compared by numerical simulations, which can provide valuable insights into the ideal design parameters. The results show that the PCE could be increased by up to 30% relative to that of the bare silicon solar cell for light incident normally on the surface.

2. Simulation and experimental methods

The two-dimensional finite-element models of the relevant cell structures (see Fig. 1) for SLARC, DLARC and surface texturing atop the silicon substrate were constructed and optimized. Arbitrary topologies, internal and external reflections and refractions, as well as polarization dependencies and dispersions, are accounted for by the TCAD software tool (Silvaco co.) to obtain exact solutions for general optical sources. In tandem with modelling optoelectronic interactions using geometric ray tracing, radiative, Shockley–Read–Hall and Auger recombinations in the bulk and surface were accounted for, plus energy balance and a range of other important (photo)physical device phenomena for photovoltaic cells; high-performance computation was carried out to obtain numerical solutions to the system of partial differential equations forming the basic semiconductor equations together with appropriate boundary conditions so that current–voltage characteristics, photogeneration rate, spectral response, etc., can be simulated (Michael and Bates, 2005). To allow meaningful comparison, identical device parameters were used, although most of them with conservative values. The SLARC is designed so that the relative phase shift between the beam specularly reflected at the upper and lower boundaries of the thin film is 180°. These two reflected beams will be cancelled by destructive interference before they exit the surface.

The required thickness of the ARC layer is given by:

$$t = \frac{\lambda}{4n_1} \tag{1}$$

where t is thickness, λ the free-space wavelength, and n_1, the index of refraction of the thin film ARC needed for complete cancellation of the two beams is given by Swatowska et al. (2011):

$$n_1 = \sqrt{(n_0 n_s)};\ (n_s > n_1) \tag{2}$$

where n_0 is the index of refraction of air (or the incident material) and n_s is the index of refraction of the substrate. n_s should be greater than n_1 to maintain the optical effectiveness of the ARC layer (Zoolfakar, 2009). To achieve zero reflectance in DLARCs, the thickness of each layer must satisfy (Ali et al., 2014):

$$t_1 = \frac{\lambda}{2\pi n_1} tan^{-1}\left\{\pm\left[\frac{(n_s - n_0)\left(n_s n_0 - n_2{}^2\right) n_1{}^2}{\left(n_s n_1{}^2 - n_0 n_2{}^2\right)\left(n_1{}^2 - n_s n_0\right)}\right]\right\}$$
$$t_2 = \frac{\lambda}{2\pi n_2} tan^{-1}\left\{\pm\left[\frac{(n_s - n_0)\left(n_s n_0 - n_1{}^2\right) n_2{}^2}{\left(n_s n_1{}^2 - n_0 n_2{}^2\right)\left(n_2{}^2 - n_s n_0\right)}\right]\right\} \tag{3}$$

where t_1 and t_2 are the optimal thicknesses, and n_1 and n_2 are the refractive indices of the top and bottom layers respectively.

Any reflected light can scatter repeatedly on a textured silicon surface, thus enhancing the absorption ratio. The coordinates of the triangular mesh rendering an arbitrarily textured surface was defined as shown in Fig. 2.

The grazing angle (propagation of the beam relative to the surface plane) is defined by parameter ANGLE (see Fig. 3). For example, ANGLE = 90 means the illumination is perpendicular to the surface. The design parameters used for the solar cell performance simulations is listed in Table 1.

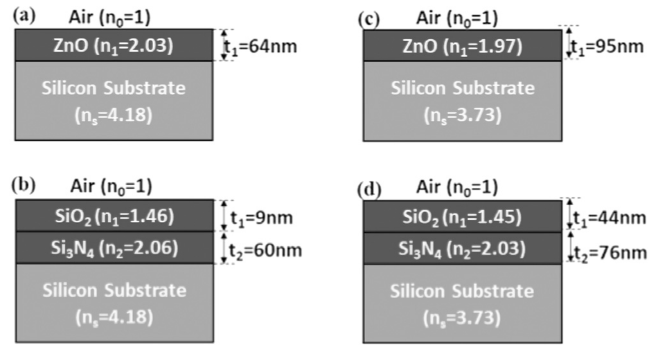

Fig. 1. Solar cell structures with (a) ZnO SLARC and (b) SiO_2/Si_3N_4DLARC at an incident wavelength of 525 nm, and (c) ZnO SLARC and (d) SiO_2/Si_3N_4DLARC at an incident wavelength of 750 nm.

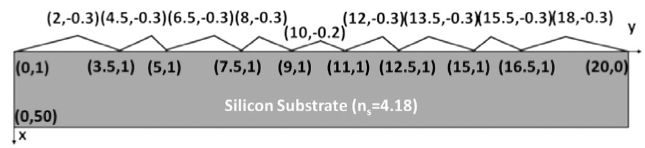

Fig. 2. Schematic of surface texturing (not to scale). The coordinates are in units of microns.

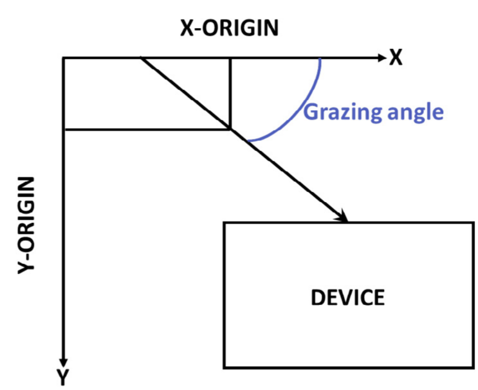

Fig. 3. Optical beam geometry.