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Computational and experimental study of a multi-layer absorptivity enhanced thin film silicon solar cell

Shima Hajimirza*, John R. Howell

The University of Texas at Austin, Department of Mechanical Engineering, USA

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ABSTRACT

We report on the computational design, fabrication and validation of a multi-layer silicon based thin film solar cell. The cell structure consists of a thin absorber layer of amorphous silicon deposited on a back-reflector aluminum layer and coated on top with ITO transparent conductive oxide. The structure is mounted on a glass substrate. We first use constrained optimization techniques along with numerical solvers of the electromagnetic equations (i.e. FDTD) to tune the geometry of the design. The resulting structure suggests that photon absorptivity in the thin film silicon can be enhanced by as much as 100% over the uncoated layer. The proposed design is then fabricated using thin film deposition techniques, along with a control sample of bare silicon absorber for comparison. AFM imaging and spectrophotometry experiments are applied to image and record the surface roughness and measure the reflectivity spectrum of the sample. Using the measured reflectivity spectrum, we then use inverse optimization to estimate the realized thin film dimensions, deposition error and unwanted oxidation volume. At the end, we use a statistical Monte Carlo analysis as a second method of verification to demonstrate that the measured spectra are in accordance with the expected curves from simulation, and to estimate the effects of fabrication error.

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1. Introduction

Amorphous silicon (a-Si) is an inexpensive choice of active layer material for thin film photovoltaic devices. Compared with crystalline silicon, a-Si has fewer stringent constraints (e.g. temperature, substrate choice, etc.) and can be deposited with smaller dimensions, and has a significantly higher solar absorption at the same thickness [1]. In addition, compared with other existing semiconductors, silicon is an abundant and well-studied material for photoelectronic uses. In spite of that, in thin film solar cells, the very small (<100 nm) thickness of silicon, and the less desirable electric properties of a-Si (compared to crystalline silicon) significantly hinder photonic absorption and photon-to-electricity conversion of the device, respectively.

Mechanical adjustments to the thin film structure can modify the optical deficiencies of silicon to a large extent. The adjustments are sometimes called “light trapping” techniques. Most commonly, light trapping is done by depositing extra layers of coating, cladding or grating on either sides of silicon. These surfaces modify the effective path length of the light in the absorbing material by the same mechanisms as in the thick film cells, as well as effects that only appear in sub-wavelength dimensions. More specifically, thin and transparent antireflective coatings (such as transparent conductive oxide layers) introduce a gradual change in refractive index to reduce surface reflectivity [2]. Furthermore, coatings designed to change the refractive index on the rear side of a device can reflect energy back through the silicon for an additional round of absorption [3–6]. Sub-wavelength plasmonic surfaces and

* Corresponding author. Tel.: +1 6187729417.
E-mail address: shimahajimirza@yahoo.com (S. Hajimirza).

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Nomenclature

c	speed of light
$C(\mathbf{x})$	cost function
$\mathbf{E}$	electric field vector
$EF(\mathbf{x})$	enhancement in the number of absorbed photons
$\bar{h}$	Planck constant
h	thickness of thin film layer
$I(\lambda)$	solar irradiance (air-mass)
N_a	number of absorbed photons
$\mathbf{x}$	parameter vector
$\alpha(\lambda)$	spectral absorptivity
ϵ''	imaginary part of the electric permittivity
λ	wavelength
Ω	wavelength range

metallic particles can produce forward scattering and localize light below the diffraction limit, effects which both lead to enhanced absorption. Metallic gratings and particles of even smaller nanoscale dimensions can use optical wavelengths to trigger surface plasmon polariton (SPP) waves or localized surface plasmon resonances (LSPR) [7–11]. When these effects are intertwined, analytical characterization of the PV conversion of the device is very challenging. Semi-analytical and computational methods are key to systematic design and study of such structures [12].

The present paper demonstrates the use of various computational techniques in the study of efficiency enhancement for thin film cells. We report on design, fabrication and verification of a simple yet efficient thin film a-Si PV structure in substrate configuration. Light entrapment in the main semiconductor layer (a-Si) is achieved via the use of a metallic back reflector layer and a transparent conductive oxide coating. The structure is plain and lacks sophisticated grating or grooming textures. In spite of that, it offers significant light trapping capability in visible and near infra-red solar spectrum, and thus enhances the overall photon absorption by a factor of 2 (i.e. %100) compared with a bare silicon layer of the same thickness. The effects of mechanisms such as metallic back reflectors and dielectric TCO coating for light trapping have been studied experimentally in several literature work such as [17–19].

Our study consists of three main parts. In the first part we exploit computational simulations and numerical methods to design the parameters of the structure. Next, we fabricate the suggested geometry in thin film deposition laboratory using Plasma Enhanced Chemical Vapor Deposition (PECVD) and sputtering, and run measurement experiments on the output sample. Estimates of surface roughness and deposition error are obtained via AFM microscopy, whereas the reflectivity spectrum of the sample is measured by spectrophotometry. Finally, the reflectivity spectra of the measured samples are compared to the simulations for verification purposes. The study in this part is quantitatively supported by the help of inverse optimization and statistical simulations.

We should emphasize that computational methods play a key role in the present study at various stages. First, we use numerical optimization to specify the parameters of the thin film structure to be made. After the sample is fabricated, we use a second and more complex inverse optimization in the verification process to explain the discrepancy between the measured and simulated spectra. More specifically, we apply an inverse analysis to numerically fit the measured spectrum through applying modifications to the target structure.

2. Thin film structure

The schematic of the thin film structure we consider in this study is shown in Fig. 1. It consists of an absorber layer of 80 nm amorphous silicon (a-Si) deposited on a layer of Aluminum back reflector, and coated on top with a layer of anti-reflective transparent conductive oxide ITO. In the process of thin film fabrication, very thin oxidized layers of Al_2O_3 and SiO_2 are formed on the layer surfaces with nominal thicknesses of 5 nm and 2 nm, respectively. The multi-layer structure is compared with a reference (control) sample that consists of a bare layer of 80 nm a-Si on the glass substrate, to quantify the absorptivity enhancement. There are two controlled parameters that determine the geometry of the cell: thicknesses of ITO and Aluminum layers:

$$\mathbf{x} = [h_{ITO}, h_{Al}] \quad (1)$$

The structure is studied in the presence of normal illumination by a solar source from the front surface side, as shown in Fig. 1 below.

Note that due to the symmetry of the structure, the source polarization is irrelevant. In numerical computations, the source is assumed to have a known irradiance $I(\lambda)$, which determines the power distribution among different wavelenghts. We consider the standardized AM1.5 solar irradiance for this purpose.

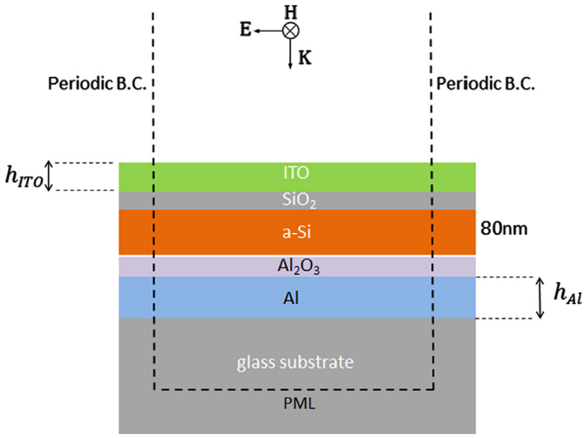

Fig. 1. Schematics of the studied multi-junction thin film cell.