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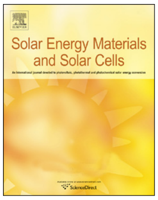

# Combined model of non-conformal layer growth for accurate optical simulation of thin-film silicon solar cells

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## ABSTRACT

In thin-film silicon solar cells textured interfaces are introduced, leading to improved antireflection and light trapping capabilities of the devices. Thin-layers are deposited on surface-textured substrates or superstrates and the texture is translated to internal interfaces. For accurate optical modelling of the thin-film silicon solar cells it is important to define and include the morphology of textured interfaces as realistic as possible. In this paper we present a model of thin-layer growth on textured surfaces which combines two growth principles: conformal and isotropic one. With the model we can predict the morphology of subsequent internal interfaces in thin-film silicon solar cells based on the known morphology of the substrate or superstrate. Calibration of the model for different materials grown under certain conditions is done on various cross-sectional scanning electron microscopy images of realistic devices. Advantages over existing growth modelling approaches are demonstrated—one of them is the ability of the model to predict and omit the textures with high possibility of defective regions formation inside the Si absorber layers. The developed model of layer growth is used in rigorous 3-D optical simulations employing the COMSOL simulator. A sinusoidal texture of the substrate is optimised for the case of a micromorph silicon solar cell. More than a 50 % increase in short-circuit current density of the bottom cell with respect to the flat case is predicted, considering the defect-free absorber layers. The developed approach enables accurate prediction and powerful design of current-matched top and bottom cell.

## 1. Introduction

In R&D of high-efficiency thin-film silicon solar cells, light management plays a substantial role [1,2]. Introducing a proper surface texture to the substrate or superstrate of a solar cell can result in enhanced light scattering and anti-reflection effect, improving light confinement in the cell. This can lead to increased photocurrent and consequently higher conversion efficiency if electrical properties of the cell remain unaffected.

Besides random textures of transparent conductive oxides (such as $SnO_2$:F [3], low pressure chemical vapour deposition–LP-CVD of ZnO:B [4], or magnetron sputtered ZnO:Al [5]) and nano-textured silver back contacts [6], artificial periodic textures have also gained much interest, showing the potential to match or even surpass the light trapping capabilities of random textures [7]. By using interference lithography, UV nano-imprint lithography, electroforming process for fabrication of large shims and UV embossing process, large area substrates with desired textures can be made on industrial scale [8–10].

In the design of efficient textures, two- or three-dimensional rigorous optical modelling is an essential tool [11–22]. For accurate determination of the optimal texture parameters realistic parameters of a solar cell have to be considered. Besides the optical properties of the layers (wavelength dependent complex refractive indices) and their thicknesses, the exact morphologies of all the textured interfaces within the device also need to be taken into account. In many publications on rigorous optical modelling of thin-film solar cells, fully conformal layer growth is considered (e.g. [14,15,18,23]) by assuming that the initial texture morphology of the substrate or superstrate is ideally transferred to all the other

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internal interfaces within the thin-film structure. However, realistic cross-sectional images of thin-film solar cells reveal that this is usually not the case [24,25]. Recently we indicated that if thicker layers are introduced or textures with high aspect ratio (ratio of vertical to lateral surface feature sizes) are used, the conformal approximation is not sufficient anymore and a combination of different growth mechanisms is required [26]. Some new approaches to the modelling of non-conformal layer growth have been researched and reported recently. These address specifically the growth of microcrystalline layers [27], or growth in general, by rounding of rectangular textures at subsequent interfaces [20], or applying one type of growth, for example, perpendicularly to the surface normal [28].

In this paper we present a combined 3-D model of non-conformal layer growth in which not only one, but a combination of two growth principles are implemented: a *conformal* and an *isotropic* one. We demonstrate on different realistic examples that the developed model, although simple and easy for implementation in optical simulations, matches with experimental the cross-sectional images of realistic structures very well and outperforms the existing single-type growth models. After calibration and verification, the growth model is integrated in rigorous 3-D optical simulations of thin-film silicon solar cells employing the COMSOL simulator, which uses the finite element method (FEM) for solving Maxwell's equations. Using the optical simulations, the sinusoidal surface texture of the substrate of a micromorph ($a$-Si:H/$\mu c$-Si:H) solar cell is optimised, with respect to increased photocurrent and, at the same time, assuring crack-free absorber layers in the device. The model enables to predict and omit the sharp valleys in the resulting textures that can lead to detrimental crack formations in semiconductor layers [27]. Using COMSOL simulations, the external quantum efficiency and short-circuit current of the micromorph device are calculated and the optimal period and height of the sinusoidal substrate texture are determined, considering all mentioned aspects.

## 2. Experimental

Masters with periodic textures were fabricated on silicon wafers using e-beam lithography and reactive ion etching. As a master with random texture standard Asahi U $SnO_2$:F transparent conductive oxide on the glass substrate was used. Ultraviolet nanoimprint lithography was employed to replicate masters on the solar cell substrates covered with a lacquer [29,30]. Amorphous solar cells were deposited using VHF-PECVD at 70 MHz with substrate temperature $T_{sub}=190\ ^\circ C$, dilution $H_2/SiH_4=2$ and pressure 0.4 mbar. Microcrystalline cells were deposited by RF-PECVD, at $T_{sub}=200\ ^\circ C$ using 200 sccm $H_2$ and 3.5–5 sccm $SiH_4$. Supporting layers: Ag, ZnO and ITO were magnetron sputtered (DC for Ag and RF for ZnO and ITO) in all types of cells. Cross-sectional images of solar cell structures were done with Hitachi IM4000 and FEI helios nanolab 400 s scanning electron microscope (SEM) equipped with a focus ion beam facility.

## 3. Modelling

### 3.1. Model of non-conformal layer growth

When building realistic optical models one of the important issues is to fit the geometry of the modelled structure to the actual structure of a solar cell as well as possible. In the case of thin-film solar cells, special attention has to be paid to the realistic representation of interfacial nano- and micro-textures in multi-layer structures, since they determine the light scattering and antireflection properties. Here we present an empirical model of layer growth which combines two growth principles: (i) *conformal* and (ii) *isotropic*. In the first principle, the morphology of the interfaces of the grown layers remains unchanged (Fig. 1a), it is simply vertically transferred from the initial substrate to the surface of the growing layer. This can be modelled by applying the growth in vertical direction of the structure only. The second type of growth principle (isotropic) describes the growth in the direction of the normal vector at any given point on the surface (Fig. 1b). Isotropy in this case refers to equal growth in all directions from each discrete point on the surface, where the resulting envelope presents the surface. Independently of the deposition method during fabrication (CVD, PVD, and condensation), a proper combination of these two types of growth was shown to result in good representation of the interface morphologies after thin-film layer depositions, except when the grown layer produces additional large texture features during growth (e.g. a thick LP-CVD ZnO or hot Ag layer). This was confirmed by the cross-sectional SEM images of various thin-film silicon solar cell structures (single junction, tandem with amorphous and microcrystalline silicon, metal layers, flat transparent conductive layers) grown on either random or periodic textures. In our model this ratio between the two growth rates (isotropic over conformal) is set by the empirical parameter called the *growth parameter* ($g$).

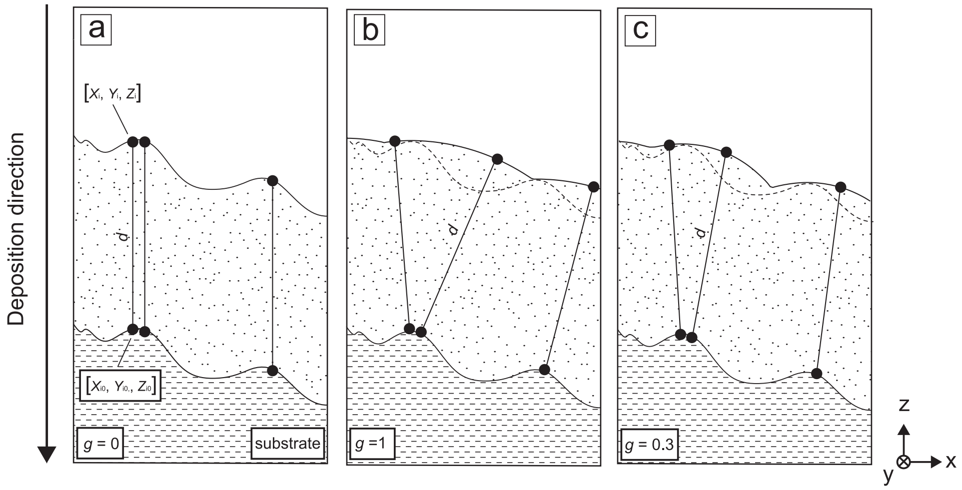

Fig. 1. Vertical cross-sections of a thin-film layer grown on a substrate as calculated by the developed 3-D growth model by considering: (a) fully conformal ($g=0$), b) fully isotropic ($g=1$) and (c) combined growth type ($g=0.3$). The dashed lines on the top surfaces in (b) and (c) indicate the reference texture obtained by conformal growth type.

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