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Prediction of defective regions in optimisation of surface textures in thin-film silicon solar cells using combined model of layer growth

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ABSTRACT

In this paper previously developed combined model of non-conformal layer growth is used to calculate positions in thin-film silicon solar cells where defective regions are expected to be formed within semiconductor layers, depending on the substrate texture. This enables omission of the textures leading to cells of poor electrical quality in the early process of optical optimisation of the cells and substrate texture design. Coupled with three-dimensional rigorous optical simulations, substrate textures are optimised with respect to high short-circuit current and defectless layer growth in micromorph silicon solar cells. Firstly, the approach of determination of defective regions is validated on realistic structures. Secondly, analysis of the effects of texture shape and of the material and the thickness of the grown layer is carried out. Thirdly, optimisation of substrate texture for micromorph type of solar cell is performed for sinusoidal, widened and semi-circular textures. Results on widened textures show, that smoothing/widening of the valleys does not always suppress the formation of defective regions in *μc*-Si:H and *a*-Si:H layers. A semi-circular type of the texture is determined to be the most appropriate for defectless absorbers in the analysed micromorph solar cells in substrate configuration, resulting also in up to 85% increase in short-circuit current of the bottom cell.

1. Introduction

In the process of improvement of the efficiency of thin-film solar cells, light management plays an important role [1,2]. Introduction of proper surface textures to superstrate or substrate of a thin-film silicon solar cell can lead to decreased front reflection and improved light scattering at the interfaces, both increasing the amount of the absorbed light within active layers of the device. This increases the generated photocurrent density and consequently the conversion efficiency of the cell.

Usually, random textures of transparent conductive oxides (TCOs), such as naturally textured SnO_2:F [3], LP-CVD (low pressure chemical vapour deposition) ZnO:B [4] or post etched magnetron sputtered ZnO:Al [5] are used to improve optical performance of the cells. Besides random, periodic textures have also shown potential to reach or even surpass optical properties of random textures if properly optimised [6–11]. Using interference or UV nano-imprint lithography large area superstrates/substrates including desired texture with high accuracy of desired texture shape can be made on large scale [12–14].

Optical modelling and simulations have been proven as an important tool in design and optimisation of new textures [6,15–17]. Nowadays, 3-D rigorous optical simulations of complete thin-film solar cell structures can be carried out in reasonable computational time. Optical optimisation of thin-film silicon solar cells on this level provides us with trends of changes of short-circuit current density (J_{SC}), which show ways to improve efficiency of solar cells. However, purely optical optimisation is not enough to build record-efficiency solar cell.

In previous publications [18–20] it was demonstrated that deposition of silicon in amorphous (*a*-Si) and especially in microcrystalline phase (*μc*-Si) on surfaces where sharp micro- or nano-valleys are present, can lead to formation of defective regions (regions of lower density of material). These regions can deteriorate electrical performance (open circuit voltage — V_{OC}, fill factor — *FF*) of solar cells significantly [9,18,21] and negate possible optical improvements obtained by introducing the texture. Some groups already aimed to avoid or soften these sharp valleys in order to achieve higher efficiencies [18,22–24]. They consider the initial surface texture of the substrate (or superstrate) surface only, and not the changes in the texture occurring due to non-conformal layer growth, which may lead to defective regions in the subsequent layers. It was previously shown [24,25] that thickness of the cell is an important factor in the determination of optimal textures as well, since defective regions can occur only later during deposition even if the initial surface does not include very sharp valleys.

This paper is organized in two parts. First we apply previously developed combined model of non-conformal growth [24] to demonstrate ability to forecast the defective regions for different textures and materials. Secondly we use the predictive power of the model in combination with 3-D rigorous optical simulations to optimise

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substrate surface textures in a thin-film silicon micromorph solar cell. This enables expansion of optical optimisation, considering occurrence of defective regions which are expected to decrease V_{OC} and FF and consequently conversion efficiency.

2. Modelling approaches

2.1. Prediction of defective regions with combined model of non-conformal growth

The proposed method for prediction of defective regions in silicon layers is based on a procedure, which has been previously used for determination of realistic change of interface textures due to deposition of thin layers (non-conformal growth) [24]. The presented method runs in Matlab and provides faster and simpler approach in comparison to previous solutions [18] and enables omission of textures, which show high potential for occurrence of defective regions at any position in active layers, already at the stage of interface design.

To describe sharpness of valleys on a surface we define the opening angle (φ) (Fig. 1). Experimental results indicated that this opening angle should be greater than 135° to avoid the formation of defective regions in microcrystalline (μc-Si:H) and amorphous (a-Si:H) silicon layers [12, 19,26]. If equal or smaller opening angle is present at the initial surface, or it is formed during the layer growth, there is a great possibility that defective regions will occur in the layer. Thus, substrates with such textures should be avoided from the beginning. Due to non-conformal layer growth it often happens that only during deposition of a layer, a surface is formed which contains smaller opening angles than on the initial substrate surface (see an example in Fig. 1 — φ_{i2}). In this case defective regions would start to form inside deposited layer and still deteriorate electrical properties [19]. Occurrence of defective regions later in deposition is expected to deteriorate solar cell in smaller degree, but here all layers including defective regions are treated as fully detrimental.

We employ the developed combined model of non-conformal growth [24] to forecast defective regions in silicon layers. In the model two types of growth: (I) conformal (vertical) and (II) isotropic (in the direction of surface normal) are combined. The ratio between both types of growth is defined by the growth parameter (g). The $g = 0$ corresponds to fully conformal, whereas $g = 1$ corresponds to fully isotropic layer growth. The value of g, which is between zero and unity, can be determined empirically from cross-sectional scanning electron microscopy (SEM) images of the analysed structures and is unique for different materials, deposition techniques and deposition parameters. Previous observations based on the analysis of SEM images of layers deposited under the same conditions at different textures showed that g can be considered as independent of the texture and of layer thickness in a certain range [24,27]. This is also an assumption in our analysis of texture optimisation.

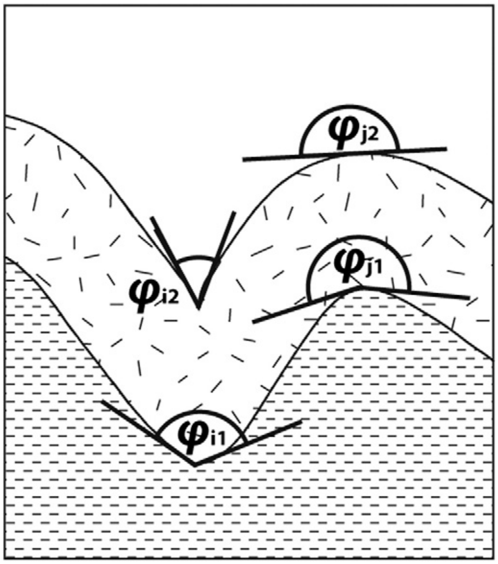

Fig. 1. Opening angle φ at different lateral positions (i and j) of the interface and at different interfaces (1 and 2).

Using the calibrated model the non-conformal growth of layers was calculated in small incremental steps (approx. every 10 nm of layer thickness). In each step, opening angles were calculated at each discrete point of the new surface. The thickness, at which critical angle ($\varphi_c = 135°$) is first found along the surface, we call critical thickness (d_c) of a layer. There, defective regions are expected to start forming for a specific type and size of the initial texture (and for certain g). This value presents the maximal thickness of a chosen layer on top of a given texture that is still expected to be defectless.

2.2. 3-D rigorous optical modelling

Presented optical simulations were done in COMSOL Multiphysics simulation software [28] where finite element method (FEM) is used for rigorous solving Maxwell's equations of electromagnetic waves. We paid special attention to meshing (discretization) of the cell structure. Multiple types of wavelength dependent meshing were combined to achieve good accuracy all over the spectrum while maintaining simulation times reasonable. To furthermore decrease computational times and resources, boundary conditions of symmetry were used to reduce the size of simulated structures to one quarter of a period [10] in both lateral directions. Realistic optical properties (wavelength dependent complex refractive indices) were considered for all layers used in simulations [29]. In calculations of J_{SC}'s ideal extraction of charge carriers from intrinsic layers of individual cells was assumed, while neglecting contributions from doped silicon layers, as this is close to actual situation within state-of-the-art solar cells [30,31].

Although FEM simulations of light propagation are rigorous, some deviations from correct realistic values of J_{SC}s are still expected to be present. Besides consideration of ideal charge carrier extraction from absorber layers only, simulation errors can be attributed to tolerances in measurement of optical properties of materials, finite discretization of the structure, discrete values of simulated wavelength of light and errors in estimation of the interface morphologies (related to the growth model). Most of these errors are difficult to evaluate quantitatively. Quality of meshing is, for example, partially reflected in the deviations between the sum of reflection, total absorption and transmission, and unity ($R + T + A = 1 \pm \delta$). In the presented simulations the errors related to δ are estimated to be <0.5% in terms of simulated J_{SC}.

3. Results

3.1. Application of the model

To demonstrate the applicability of the model to forecast defective regions we simulated the growth of microcrystalline silicon layer on top of naturally textured LP-CVD ZnO. The cross-sectional SEM images of layers were taken from the literature [20]. Fig. 2A and C shows two SEM images of actually deposited microcrystalline (μc-Si:H) silicon layers of different density. Case A shows situation in porous μc-Si:H layer and case C shows dense μc-Si:H layer. Dark region in these images presents the areas of material of lower density — defective regions. Fig. 2B and D shows local opening angle at the surface throughout the layer as predicted with the combined model of non-conformal layer growth. Darker regions show areas of low opening angles, where defective regions are expected to occur within the cell. The comparison of Fig. 2A and C to B and D, respectively, shows good agreement between the actual defective regions (in A and C) and areas with high