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On the interplay of interface morphology and microstructure of high-efficiency microcrystalline silicon solar cells



Asman Tamang^a, Hitoshi Sai^b, Vladislav Jovanov^a, Sardar I.H. Bali^a, Koji Matsubara^b, Dietmar Knipp^{a,*}

^a Research Center for Functional Materials and Nanomolecular Science, Electronic Devices and Nanophotonics Laboratory, Jacobs University Bremen, Bremen, Germany

^b Research Center for Photovoltaic Technologies, National Institute of Advanced Industrial Science and Technology (AIST), Ibaraki, Japan

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ABSTRACT

The relationship between light trapping and microstructure of high-efficiency microcrystalline silicon thin-film solar cells on honeycomb textured substrates is investigated by experiments, optical simulations and analytical calculations. The solar cells realized on the honeycomb textured substrates exhibit short circuit current of 30 mA/cm² and energy conversion efficiencies exceeding 11%. The microstructure of the solar cells is limited by the formation of so called "cracks" in the film, which negatively affect the short circuit current, fill factor and open circuit voltage. The formation of cracks is studied by transmission electron microscopy, optoelectrical measurements and simulations of the 3D morphology of the solar cell. Furthermore, a simple analytical model is presented to calculate the critical thickness at which cracks are formed. Both models are compared to experimental results. Guidelines are provided on how to avoid the formation of cracks in microcrystalline silicon films on the textured substrates while maximizing the light trapping properties.

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1. Introduction

Light trapping and photon management are imperative in improving the short circuit currents of microcrystalline thin-film silicon solar cells [1–3]. The short circuit current is commonly increased by texturing the contacts of the thin-film solar cells [1–25]. However, in order to achieve high short circuit currents, the photo-generated charges have to be efficiently collected. Furthermore, high fill factors and open circuit voltages are required to realize high energy conversion efficiencies. Unfortunately, all these parameters can be negatively affected by recombination centers, which are formed during the growth of the microcrystalline silicon film [2,14,26–30]. A high concentration of recombination centers occurs in regions with reduced structural order. The formation of such regions is often referred to as a "crack formation". Such cracks might occur if the material is prepared on textured substrates, while microcrystalline silicon films prepared on flat or smooth substrates do not exhibit voids or cracks. By increasing the roughness of the substrates the concentration of cracks in the film is increased [29]. Material characterization by secondary ion mass spectrometry (SIMS) reveals that the oxygen concentration in the

* Corresponding author. E-mail address: dietmarknipp@gmail.com (D. Knipp). crack region is increased which results in reduced charge collection efficiency, lower fill factor and open circuit voltage [29].

In this study, we describe a mathematical procedure to predict the crack formation and propagation, and present a simple equation that allows for calculating a critical thickness up to which no cracks are formed. The calculations are compared to experimental results. Microcrystalline silicon solar cells in substrate configuration prepared on honeycomb textured substrates are used for this study. Microcrystalline silicon single junction solar cells and triple junction solar cells prepared on honeycomb textured substrates hold record energy conversion efficiencies of 11.8% [3] and 13.6% (14.5% initial) [31], respectively.

2. Device fabrication

In the first step of the fabrication process, the periodically textured back contact/reflector of the solar cells is realized by etching a honeycomb pattern in a thermally oxidized silicon wafer through a hexagonally arranged etch-mask with the opening of 700 nm. The etched substrates exhibit a height to period ratio of 0.25. The period of the substrate (*P*) is defined as the distance between two tips of the honeycomb texture (Fig. 1(c)), while the height of the substrate (*H*) represents the difference between the maximum and the minimum point of the substrate (Fig. 1(d)). In



Fig. 1. Top views of honeycomb textured silver back reflector (a) before and (b) after the deposition of 3 µm thick microcrystalline silicon. The period of the surface texture (*P*) is 3 µm, while the height (*H*) is 0.75 µm. Schematic cross-sections of the µc-Si:H solar cells for (c) direction *A* and (d) direction *B*.

the next step, a double layer consisting of silver (Ag) and gallium doped zinc oxide (ZnO:Ga) is sputtered on top of the textured substrate. A schematic top view of the substrate is shown in Fig. 1 (a). Afterwards, a microcrystalline silicon (μ c-Si:H) p-i-n diode is deposited on top of the ZnO:Ga layer using a plasma enhanced chemical vapor deposition (PECVD) process [3,19–21]. Wide band gap silicon oxide (Si_{1-x}O_x) layer is used as p-layer of the p-i-n diode to minimize the optical loss in the p-layer [2,3,12,14,21]. The p-layer and n-layer of the p-i-n diode have a thickness of 10 nm and 30 nm, respectively. Finally, a 70 nm thick indium tin oxide (In₂O₃:Sn, ITO) layer is sputtered on top of the silicon film to act as a front contact. Further details on the fabrication of the microcrystalline silicon solar cells on the honeycomb textured metal back reflectors are given in the literature [3,14,21]. A schematic top view of the solar cell is shown in Fig. 1(b).

3. Modeling of silicon thin-film solar cells

In order to investigate the crack formation and optics, the interface morphologies of the solar cells have to be properly calculated.

3.1. Interface morphologies of silicon thin-film solar cells

A 3D morphological algorithm is used to model the etching of the substrate and deposition of the solar cell. The calculated top views of the textured substrates before and after the deposition of the microcrystalline silicon films are shown in Fig. 1(a) and (b), respectively. A good agreement is obtained between the calculated (Fig. 1) and the measured surface morphology [21]. The 3D morphological model assumes that the etching of the silicon oxide film and the deposition of the silicon film take place in the direction of the local surface normal [25,32,33]. To simulate the etching process, a hexagonally arranged etching mask with an opening of 700 nm is used. This dimension is the same as for the fabricated substrates. The surface morphology of the silicon film is calculated for each substrate point depending on the angle between the local surface normal and substrate normal. The silicon film thickness is equal to the nominal film thickness. d. if the local surface normal is parallel to the substrate normal. If the local surface normal is orthogonal to the substrate normal, the thickness is reduced by the direction factor (K), so that the thickness is given by $K \times d$. In this study, a direction factor of 0.75 is used. This value is determined by a comparison of measured and simulated surface morphologies of microcrystalline silicon films prepared by the Institute of Photovoltaics of the Research Center Jülich [33]. As a reference, the direction factor for device-grade amorphous silicon films is very close to 1 [25,32-34]. This is supported by several publications which show the surface coverage of amorphous silicon films on micro and nanowire geometries [12,34,35]. Further details on the deposition algorithm are given in the literature [32,33].

The direction factor depends on the conditions used for the deposition of the silicon films. Changing the gas composition during the deposition, the pressure in the deposition chamber and the deposition power change the direction factor. Kim et al. determined a direction factor of 0.6 ± 0.1 [30] for microcrystalline silicon films prepared by Python et al. [28, 29]. As an alternative, Sever et al. for the same experimental data [28,29] proposed a

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