Influence of interface morphologies on amorphous silicon thin film solar cells prepared on randomly textured substrates

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ABSTRACT

The influence of the interface morphologies on amorphous silicon thin-film solar cells prepared on randomly textured substrates was studied. A simple three-dimensional geometrical model was developed to describe the surface morphology of amorphous silicon films and thin-film solar cells. The simulated surface morphologies are confirmed by experimental measurements. A detailed understanding of the interface morphologies is required to gain insights in the light-trapping of silicon thin-film solar cells on randomly textured substrates and derive strategies to improve the light-trapping properties. The morphology of amorphous silicon solar cell layers is calculated by using atomic force microscope scans of the randomly textured substrates and the thickness of layers as input data. The influence of the interface morphologies on the surface roughness, average film thickness and size of surface textures is investigated. Finally the influence of these parameters on the light-trapping and optical losses is discussed.

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1. Introduction

In order to maximize the conversion efficiency of thin-film solar cells the electrical and optical losses have to be minimized. In the case of low temperature amorphous silicon thin-film solar cells, the silicon material exhibits a low charge carrier diffusion length when the thickness of the solar cell is limited to a couple of hundreds of nanometers. In order to achieve high short circuit currents for such thin solar cells, light-trapping or photon management is necessary. The aim of light-trapping is to maximize the absorption of light in the thin absorber layer of the solar cell. Randomly textured transparent conductive oxides (TCO) are commonly used in silicon thin-film solar cells as front contacts. The surface textures of the transparent conductive oxides reduce reflection losses and increase scattering/diffraction of the incident light [1–8]. Randomly textured TCO can be realized by wet etching of sputtered zinc oxide (ZnO) films, direct deposition of textured zinc oxide by low pressure chemical vapor deposition (LPCVD) or tin oxide films by atmospheric pressure chemical vapor deposition (APCVD) [1–8].

Optical simulations and experimental results reveal that enhanced light-trapping is achieved when both front and back contacts are textured [9,10]. Texturing of the back contact is achieved by propagation of front contact surface textures during solar cell deposition. It is commonly assumed in literature that the back contact surface textures are an exact replica of the front contact textures [9,11–15]. However, experimental measurements reveal significant differences between the front and back contact morphology of silicon thin-film solar cells [10,16–20]. Fig. 1 exhibits a cross section of an amorphous silicon thin-film solar cell in superstrate configuration. The interface morphology of the front and back contact surface textures in Fig. 1 are based on experimentally measured surface profiles.

Light-trapping in silicon thin-film solar cells is determined by the front and back contact morphology. The front contact surface textures determine the incoupling and scattering/diffraction of the incident light. The back contact textures determine the scattering/diffraction of longer wavelength light and the optical losses in the metal back contact. In order to gain insight in the light-trapping and optics of thin-film solar cells, a detailed knowledge of the front and back contact morphology is required. The front contact morphology is determined by the surface textures of the TCO. On the other hand, the back contact morphology is determined by the front contact textures and the formation of the amorphous silicon solar cell layers. In this manuscript we investigate the interface morphologies of the solar cell and their influence on light-trapping. The surface coverage algorithm used to determine the interface morphologies is introduced in Section 2. In Section 3 the properties of the solar cell
front contact are described. The back contact morphology is presented in Section 4. Finally, the light-trapping in amorphous silicon thin-film solar cell is discussed in Section 5 before summarizing the results in Section 6.

2. Modeling surface morphologies of amorphous silicon thin films on textured substrates

Plasma enhanced chemical vapor deposition (PECVD) is the standard process used in solar cell industry for the fabrication of low temperature amorphous silicon solar cells [1,2,6,7,11,21]. The growth conditions can be varied between physical vapor deposition (PVD) conditions and chemical vapor deposition (CVD) conditions [22–24]. PVD-like growth conditions result in amorphous silicon films, which exhibit a columnar microstructure and, consequently, a high defect density. On the other hand, CVD-like growth conditions result in films with much lower defect density, which is essential for the fabrication of amorphous silicon solar cells with good electrical properties. The PECVD process with CVD-like growth conditions exhibits a low sticking coefficient, which results in amorphous silicon films with excellent surface coverage. The growth of silicon thin-film solar cells is a complex process especially for microcrystalline silicon material [25]. However, for the deposition of low temperature amorphous silicon solar cells it can be simply assumed that the silicon film grows in the direction of the local surface normal (Fig. 2(b)). A schematic sketch of the film growth is shown in Fig. 2.

Fig. 2(a) exhibits the formation of an amorphous silicon film according to the standard assumption [9,11–14]. The surface morphology of the amorphous silicon film is an exact replica of the substrate morphology and the deposited film thickness is equal for each position of the substrate. The film formation in the direction of the local surface normal is shown in Fig. 2(b). The surface morphology of amorphous silicon film is different from the substrate, which results in different film thicknesses at different locations. So far the influence of the interface morphology was rarely considered when discussing the optical and electrical properties of silicon thin film solar cells prepared on the randomly textured substrates. In order to overcome this shortcoming, a three-dimensional surface coverage algorithm was developed. The surface coverage algorithm can generate silicon film morphologies under the assumption that the silicon film grows in the direction of the local surface normal by using the surface morphology of randomly textured substrate and film thickness as input data. The surface normal cannot be defined for the peak and valley points of the substrate. For each peak point of the substrate the surface coverage algorithm assumes an equidistant surface which connects to the film surface predicted by substrate points for which the surface normal is defined. In the vicinity of the substrate valley points, for every \( x \)- and \( y \)-coordinate several film surface points can be calculated and only highest surface points are selected.

In order to verify the developed 3D surface coverage algorithm, the morphologies of amorphous silicon films deposited on two different randomly textured substrates (Asahi U substrate and sputtered and wet etched ZnO substrate) were measured and simulated. Amorphous silicon and tandem solar cells prepared on these substrates exhibit high conversion efficiencies [1,26]. In the first step, the surface morphologies of the substrates were measured by using atomic force microscopy (AFM). In the next step, 300 nm thick amorphous silicon films were deposited on the substrates and measured by AFM. The amorphous silicon films were deposited by a PECVD process with deposition temperature of 260 °C using a gas mixture of silane and hydrogen. A film thickness of 300 nm was selected to be consistent with the thickness of a typical amorphous silicon solar cell diode, where the p-layer is 10 nm thick, i-layer is 280 nm thick and n-layer is 10 nm thick. An alignment procedure using laser markers was established to measure the morphology of amorphous silicon film for the same area as for the substrate measurement. In the final step, the morphologies of the silicon films were calculated for both substrates.

Fig. 3(a) exhibits the measured line scans of an Asahi U substrate and a 300 nm thick deposited amorphous silicon film and line scan extracted from the calculated silicon film morphology.
The simulated surface profile resembles the measured surface profile. Fig. 3(b) exhibits the measured and simulated line scan of a 300 nm thick amorphous silicon film deposited on a sputtered and wet etched ZnO substrate. Again the simulated morphology of the silicon film matches the measured morphology very well. The good agreement between the measured and simulated morphologies confirms that the developed 3D surface coverage algorithm can accurately predict the surface and interface morphologies of low temperature amorphous silicon solar cells.

3. Front layers of the solar cell

In order to characterize the solar cell front layers, the surface coverage algorithm was used to determine the morphologies of p-layer and i-layer of a typical amorphous silicon cell. It was assumed that the film formation of the p-layer and i-layer is comparable. AFM scans of Asahi U (Fig. 4(a)) and etched ZnO (Fig. 5(a)) substrate were used as input data for the calculations. The thicknesses of the p- and i-layer (nominal values) were chosen to be 10 nm and 280 nm, respectively. Hence the thicknesses of the p- and i-layer are consistent with dimensions of typical amorphous silicon solar cells.

The morphology of an Asahi U substrate is measured by atomic force microscopy and it is shown in Fig. 4(a). The scan can be described by the height function \( h(x,y) \), where \( x \) and \( y \) represent the \( x \)- and \( y \)-coordinates. The Asahi U type substrate can be characterized by the random arrangement of pyramid-like features with diameters in the range from 50 nm to 400 nm. The height of pyramid-like features ranges from 90 nm to 300 nm. The simulated morphology of the p-layer is presented in Fig. 4(b). The morphology of the p-layer shows almost no difference compared to the substrate. However, the difference can be determined by calculating the thickness gain of the p-layer, which is given by:

\[
\Delta d_p(x, y, d_p) = \frac{h_p(x, y, d_p) - h(x, y)}{d_p} - 1
\]

where \( d_p \) is the nominal film thickness of the p-layer, \( h_p(x, y, d_p) \) and \( h(x, y) \) are height functions of the p-layer and substrate, respectively. The thickness gain depends on the surface area of the substrate and thickness of the deposited film. For a smooth (flat) substrate the deposited film thickness is equal to the nominal film thickness and the thickness gain is zero. Textured substrates exhibit an increased surface area and the actual film thickness is larger than the nominal thickness. Exceptions are substrate peak points where the deposited thickness is equal to nominal thickness. The thickness gain of the p-layer for the Asahi U substrate is shown in Fig. 4(c). The red areas in Fig. 4(c) mark the regions for which the thickness gain is 50% or larger. The largest gain in the thickness is observed for the valley areas of the substrate. The lowest gain is observed for the peak areas of the substrate. The surface morphology of the simulated i-layer is presented in Fig. 4(d) and it is significantly different from the substrate (Fig. 4(a)). The thickness gain of the i-layer was calculated respective to the p-layer:

\[
\Delta d_i(x, y, d_i) = \frac{h_i(x, y, d_i) - h_p(x, y, d_p)}{d_i} - 1
\]

where \( d_i \) is the nominal thickness of the i-layer, \( h_i(x, y, d_i) \) and \( h_p(x, y, d_p) \) are the height functions of the i-layer and p-layer, respectively. The thickness gain of the i-layer is shown in Fig. 4(e). A comparison of thickness gain of the p-layer and i-layer shows that the thickness gain is lower for the i-layer, which is caused by reduced surface area. However, the absolute increase in the thickness for the i-layer is larger than for the p-layer.

Fig. 5(a) exhibits the atomic force microscopy scan of the sputtered and etched zinc oxide substrate. The surface of the etched ZnO substrate can be characterized by crater-like features with diameters in the range from 500 nm to 2000 nm. The depth of the crater-like features ranges from 100 nm to 500 nm. The simulated morphologies of p-layer and i-layer are shown in Fig. 5(b) and (d), respectively. Again, the morphology of the p-layer shows almost no difference compared to the substrate, while the morphology of i-layer is slightly different from the substrate. The thickness gains of p-layer and i-layer were calculated accordingly to Eq. (1) and Eq. (2) and presented in Fig. 5(c) and (e), respectively. The thickness gains for p-layer and i-layer deposited on etched ZnO substrate are smaller than for Asahi U substrate. The surface textures of etched ZnO substrate are much larger than for Asahi U substrate and therefore the change of the surface area and thickness gain is much smaller for the same deposited film thickness.

The results in Figs. 4 and 5 show that the actual thickness of the p- and i-layer is larger than the nominal film thickness, due to the formation of the amorphous silicon film on the surface. The gain in the film thickness cannot be detected in typical thickness measurements by surface profilers. The tip of a surface profiler is relatively large compared to the lateral dimensions of the surface textures. Therefore, the tip of the profiler detects only
the topmost surface levels where the deposited film thickness is equal to nominal thickness [27]. Consequently, the measured thickness does not take any filling of valleys into account. The effective thickness of solar cell layers can be obtained only by atomic force microscope measurements. To compare the thickness of the p-layer on the Asahi U and etched ZnO substrate, an average (effective) thickness of the p-layer was calculated. For the deposited film thickness of 10 nm, an effective thickness of 12.2 nm and 10.9 nm was calculated for the Asahi U and the etched ZnO substrate, respectively. The effective thickness of the p-layer depends on the substrate morphology and the deposited thickness of p-layer. The increased thickness of the p-layer results in increased absorption of the light in the p-layer. This is important for shorter wavelength light (less than 450 nm), which gets absorbed in the front of the solar cell. Consequently, the quantum efficiency for shorter wavelengths will be reduced. On the other hand, the increased thickness of the i-layer results in the increased absorption of longer wavelengths light (longer than 550 nm). Therefore, the quantum efficiency for longer wavelengths will be increased. The effective thickness gain of the i-layer for the Asahi U and etched ZnO substrate was calculated. The effective thickness gain of the i-layer for the Asahi U and etched ZnO substrate is shown in Fig. 6.

Fig. 6 exhibits the effective thickness gain of the i-layer as a function of the deposited thickness of the i-layer. The p-layer thickness was varied as a parameter. The effective thickness gain strongly depends on the type of substrate used for the deposition of the solar cell. The effective thickness gain of the i-layer for the Asahi U substrate is presented in Fig. 6(a). For very thin i-layers the effective thickness is more than 15% larger than the deposited film thickness. The effective thickness gain drops with increased thickness of p-layer and i-layer. For a solar cell with a p-layer thickness of 10 nm and i-layer of 280 nm, effective thickness gain is 11.5% which results in an effective thickness of the absorber layer of 312 nm. Fig. 6(b) exhibits the effective thickness gain of i-layer for an etched ZnO substrate. For very thin absorber layers the effective thickness is only 9% higher than the deposited film thickness. For etched ZnO substrate the effective thickness gain also drops with increased thickness of deposited p-layer and i-layer. However, the change in the effective thickness gain is much smaller compared to the Asahi U substrate. For a solar cell with a p-layer of 10 nm and i-layer of 280 nm, effective thickness gain is 8.2% which results in an effective thickness of the i-layer of 303 nm.
4. Back contact morphology

The back contact morphology depends on the front contact textures and the thickness of the solar cell diode (Figs. 4 and 5). In order to quantify the influence of the solar cell diode thickness on the back contact surface textures and roughness, the surface coverage algorithm was used to generate back contact morphologies for Asahi U and etched ZnO substrate for several different thicknesses. The calculated back contact morphologies were used to determine the average feature size and the root mean square (rms) roughness of the back contact surface. The size of surface textures was determined by calculating the auto correlation function of the surface morphologies. In the first step, the auto correlation function (ACF) was calculated by:

\[
ACF(l_x, l_y, d) = \lim_{A \to \infty} \int \int h(x, y, d) \times h(x + l_x, y + l_y, d) \times dx \times dy
\]

where \(d\) is nominal thickness of the p–i–n diode and \(h(x, y, d)\) is the height function of the simulated back contact morphology. Since the surface textures are random a 2-D ACF can be transformed into a 1-D radial function. The ACF for the Asahi U substrate and etched ZnO substrate are shown in Fig. 7.

\[
ACF(l) = \sigma^2 \exp\left(-\frac{l^2}{L_c^2}\right)
\]

where \(\sigma\) presents the root mean square deviation of the heights and \(L_c\) the auto correlation length. The correlation length was determined by fitting the calculated ACF of the simulated surface morphology with the Gaussian distribution. The size of the pyramids-like features of the Asahi U substrate and the size of the crater-like features of the etched ZnO substrate is given by:

\[
L_f = \sqrt{2} \times L_c
\]

The size of the surface textures for Asahi U substrate and etched ZnO substrate are plotted as a function of silicon diode thickness and presented in Fig. 8. The extracted diameters of the
pyramids and craters are in good agreement with image segmentation approaches used to determine the feature size for Asahi U and etched ZnO substrate [28]. In order to quantify the influence of the silicon diode thickness on the roughness of the surface, the root mean square roughness was calculated for generated back contact morphologies. The calculated rms roughness of the Asahi U and etched ZnO substrate are shown in Fig. 8. Fig. 8 also exhibits measured back contact roughness from Section 2 and from [26] for amorphous silicon solar cells deposited on Asahi U and etched ZnO substrates.

Fig. 8(a) shows the roughness and feature size of the back contact for the solar cells deposited on Asahi U substrate as a function of the silicon diode thickness. The roughness drops with increasing thickness, while the average diameter of the pyramid-like features increases. The Asahi U type substrate exhibits an rms roughness of 41 nm and average feature size of 240 nm. For a typical solar cell thickness of 300 nm back contact roughness is 34 nm and average pyramid diameter is 350 nm. The rms roughness and crater diameter for the etched ZnO substrate as a function of solar cell thickness is presented in Fig. 8(b). The roughness of the etched ZnO substrate is 116 nm and it is much higher than the Asahi U substrate. The average crater diameter for the ZnO substrate is close to 960 nm. For the etched ZnO substrate the roughness also drops with increased thickness of solar cell. However, the drop is significantly smaller than for the Asahi U substrate. The rms roughness of a 300 nm solar cell deposited on the etched ZnO is 114 nm. The average crater diameter remains almost constant irrespective of the thickness of the solar cell. For 300 nm thick solar cell the average crater diameter is 948 nm and for 500 nm thick solar cell crater diameter is 952 nm.

5. Discussion

The short circuit current density of a silicon thin film solar cells depend strongly on an efficient light-trapping scheme. In order to maximize the short circuit current the front and the back contact have to be textured. Determining the optimal feature size for light-trapping in thin-film solar cells is complex. Most research groups focus their investigation either on the front or back contact. However, the influence of the front and back contact of the thin-film solar cell cannot be easily decoupled. The developed 3D surface coverage algorithm allows for a detailed and accurate description of the interface morphology of low temperature amorphous silicon solar cells. Consequently, the influence of the interface morphology on the solar cell properties and light-trapping can be determined. For this purpose, two different types of random textured substrates
A rather different. The etched ZnO substrate is characterized by layers have to be considered. When optimizing the light-trapping of thin-film solar cells prepared on Asahi U type substrates, the different front and back contact morphologies and the increased thickness of solar cell layers. For a typical amorphous silicon solar cell deposited on an etched ZnO substrate with 10 nm p-layer and 280 nm i-layer, p-layer thickness is increased by 9% and the i-layer thickness is increased by 8.2%. Solar cells prepared on substrates with surface features much larger than the deposited film thickness, exhibit only small difference between the front and back contact morphology. However, the increased thickness of solar cell layers has to be considered when optimizing the light-trapping.

Fig. 8. Calculated and measured root mean square roughness and estimated feature size of back contact textures for amorphous solar cells deposited on (a) Asahi U and (b) etched ZnO substrate.

were analyzed: the Asahi U type substrate and sputtered and wet etched ZnO substrate.

The Asahi U type substrate is characterized by rather small pyramid-like features with average diameter of 240 nm and root mean square roughness close to 41 nm. If the thickness of the prepared film is comparable to the size of surface features a distinct change of the surface morphology is observed. As a consequence the rms roughness drops from 40 nm to 34 nm for a 300 nm thick solar cell. Therefore, the back contact surface is smoother compared to the front contact. Furthermore, the average diameter of the pyramids increases as a function of the solar cell thickness. As a consequence the back contact features are larger than the front contact features. The average diameter of the back contact features for a 300 nm thick solar cell is close to 350 nm. Another important parameter is the effective thickness of the solar cell layers. For a typical solar cell with nominal thickness of 10 nm for p-layer and 280 nm for i-layer, thickness increase of 22% is calculated for the p-layer and 11.5% for the i-layer. The increased thickness of the i-layer leads to increased quantum efficiency of the solar cell. On the other hand, the increased thickness of the p-layer results in higher optical losses in the p-layer. When optimizing the light-trapping of thin-film solar cells prepared on Asahi U type substrates, the different front and back contact morphologies and the increased thickness of solar cell layers have to be considered.

The situation for the sputtered and wet etched ZnO substrate is rather different. The etched ZnO substrate is characterized by large crater-like features with an average diameter of 960 nm and root mean square roughness of 116 nm. The surface features are much larger than the thickness of the deposited film and consequently the morphology of the back contact is comparable to the morphology of etched ZnO. Hence, the crater size and roughness of the front and the back contact are similar. The increase of the thickness of the solar cell layers is smaller compared to Asahi U substrates. For a typical amorphous silicon solar cell deposited on an etched ZnO substrate with 10 nm p-layer and 280 nm i-layer, p-layer thickness is increased by 9% and the i-layer thickness is increased by 8.2%. Solar cells prepared on substrates with surface features much larger than the deposited film thickness, exhibit only small difference between the front and back contact morphology. However, the increased thickness of solar cell layers has to be considered when optimizing the light-trapping.

6. Summary

The influence of the interface morphology on the solar cell layers was investigated. In order to predict the interface morphology of low temperature amorphous silicon solar cells a 3D surface coverage algorithm was developed. The algorithm assumes that amorphous silicon deposited on randomly textured substrate grows in direction of the surface normal. This assumption is valid for the fabrication of low temperature amorphous silicon solar cells. The surface coverage algorithm was confirmed by AFM measurements of silicon thin film morphologies on Asahi U and etched ZnO substrates. A good agreement between the calculated and the measured surface profiles was observed. The 3D surface coverage algorithm was used to determine the interface morphologies of amorphous silicon solar cell layers and the influence on the light-trapping was investigated. If the size of the surface textures is comparable to the thickness of the deposited silicon film, the morphology of the back contact is distinctly different from the front contact morphology. The back contact feature size is larger and the roughness of the back contact is reduced. Also, the effective thickness of the solar cell layers is larger than the nominal thickness. If the size of surface features is larger than the thickness of the silicon film, the back contact morphology exhibits only smaller differences compared to the front contact morphology. The feature size and roughness of the back contact are comparable to the front contact textures and roughness. In this case, only a small increase of the thickness of the solar cell layers is observed. Determining the interface morphology of solar cells allows for the further understanding of the light-trapping and the development of novel light-trapping structures.

References


