The impact of intermediate reflectors on light absorption in tandem solar cells with randomly textured surfaces

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The impact of dielectric intermediate reflectors on the light absorption in the top cell of an *a*-Si:H/μc-Si:H tandem solar cell comprising randomly textured surfaces was investigated by rigorous diffraction theory. Despite the strong light scattering, we found Fabry–Pérot oscillations for the absorption with a decreasing modulation for an increasing thickness of the intermediate layer, a larger oscillation period when compared to thin films and a homogenization of the absorption profile. Optimized intermediate reflectors generate an absorption enhancement in the *a*-Si:H film, which varies between a factor of 2 and more than 3 for wavelengths of strong and weak absorption, respectively. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3142421]

The optimization of energy conversion in thin-film solar cells based on hydrogenated amorphous (*a*-Si:H) and microcrystalline (μc-Si:H) silicon is a very promising way for efficiency enhancement in photovoltaic technology. Such cells are made from sustainable and low-cost materials. Since the technology is compatible with large area processing, *a*-Si:H and μc-Si:H based solar cells have a great potential. Due to the small intrinsic diffusion length of the generated electron-hole pairs in *a*-Si:H, the thickness of the absorber layer is limited to a few hundred nanometers. Therefore, photons, particularly at long wavelengths, are only poorly absorbed in thin-film *a*-Si:H solar cells. In tandem structures consisting of an *a*-Si:H top and a μc-Si:H bottom cell,[1] the *a*-Si:H top cell typically limits the output current density of the device. Thus, concepts for photon management are required to increase the absorption in the *a*-Si:H top cell. Potentially the most promising approach is the incorporation of randomly textured surfaces.[2] In addition, intermediate reflector layers may be integrated between the *a*-Si:H and the μc-Si:H layer.[3,4] This reflector should have a low refractive index and a matched thickness to increase the amount of light trapped in the *a*-Si:H top cell in the long-wavelength regime at a low electrical resistance.

A full theoretical analysis has to take into account both, the randomly textured surface and the intermediate layer, to design a tandem solar cell with optimized efficiency. While the analysis of the flat layer stack of a tandem solar cell can be reasonably done, the incorporation of randomly textured surfaces constitutes a significant challenge.[5–8] In earlier works techniques were developed to describe the light scattering properties of such surfaces; each with certain limitations. The theory by Beckmann and Spizzichino,[9] for example, uses the Kirchhoff approximation, which fails if the significant feature sizes of the surface are comparable to the wavelength. It also neglects multiple scattering. Other techniques such as those based on the Ewald–Oseen extinction theorem[10] are usually only applied to perfectly conducting interfaces. Consequently, the analysis of a complex device such as a tandem solar cell that includes rough surfaces and an intermediate reflector is usually done by applying techniques that impose strong approximations and/or assumptions on the structure as, for example, periodic gratings.[11]

We apply here an assumption-free rigorous diffraction theory, namely the finite-difference time-domain (FDTD) method, to consider this problem.[12] Textures retained in the FDTD method were taken from atomic force microscope images of a real device.[13] It was fabricated by etching a 1000 nm thick ZnO layer deposited on a glass substrate with HCl. The profile taken for all subsequent simulations is shown in Fig. 1(d). The size of the surface retained in the simulations was $7\times7\ \mu m^2$. Such size is sufficient to exclude that any result obtained can be attributed to the singular implementation of the surface morphology, instead the results are generic peculiarities of the structure. Different layer stacks with increasing complexity were studied starting with an *a*-Si:H top cell capped with an intermediate layer of varying thickness. Subsequent to this structure, air or μc-Si:H layers with either 40 nm or infinite thickness were assumed. This allows to analyze the impact of an intermediate reflector on the absorption in a tandem solar cell with randomly textured interfaces at various stages.

The sequence of layers used in the simulation is shown in Fig. 1(e). Below the ZnO surface an *a*-Si:H layer with a fixed thickness of 250 nm was assumed. Optically this layer represents the *a*-Si:H solar cell. The variable intermediate layer thickness is denoted by h_{IL}. Refractive index of this layer was representatively assumed as $n=2$. We discriminate the three following scenarios. (I) No additional layer was placed below the intermediate reflector. (II) An additional μc-Si:H layer with a thickness of 40 nm was placed between the intermediate reflector and air. (III) The thickness of the μc-Si:H layer was chosen to be infinite.

The latter structure reflects the layer stack for practical applications disregarding the finite thickness of the μc-Si:H layer. This is reasonable because in real devices the μc-Si:H layer is sufficiently thick to assure complete absorption of the relevant photons after a dual passage. Therefore, no further interference phenomena at the wavelengths of interest will occur.

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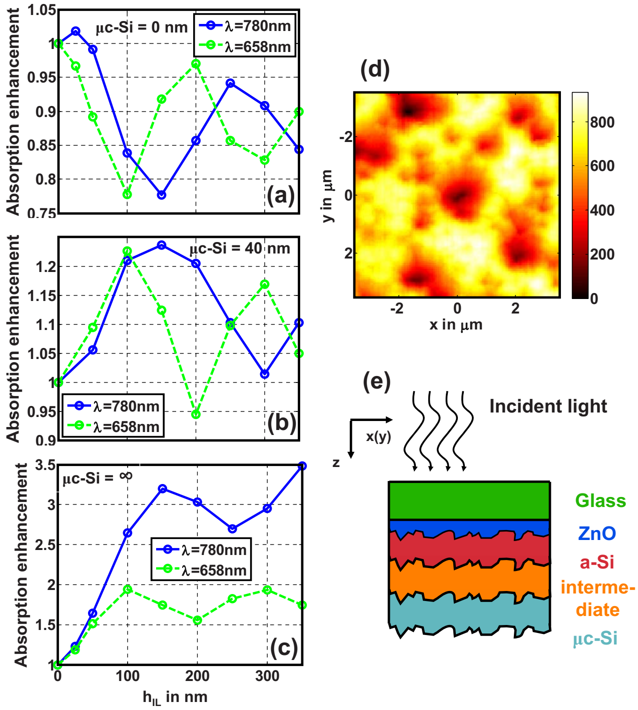

FIG. 1. (Color online) Absorption enhancement in the a-Si:H layer of a tandem solar cell as a function of the thickness of the intermediate layer, h_{IL}, for two relevant wavelengths (blue solid line denotes $\lambda=780$ nm and green dashed line denotes $\lambda=658$ nm). (a) Cell consisting of a 250 nm a-Si:H layer below a randomly textured ZnO film deposited on a glass substrate. (b) An additional 40 nm layer of μc-Si:H was sandwiched between the intermediate layer and air. (c) The μc-Si:H layer has infinite thickness. (d) Surface profile in nanometer retrieved from an atomic force micrograph of a fabricated solar cell. (e) Schematic of the layer stack.

For computing the absorption, the light evolution through the systems was simulated using the FDTD method. It was assumed that the structure is illuminated by a linearly polarized, normally incident plane wave from the substrate side. The positive z axis defines the propagation direction. Two wavelengths (780 and 658 nm) were chosen, which represent the spectral domain where the intermediate reflector is expected to have its greatest impact on the top cell. It corresponds to the spectral range of the transition from a reasonably good to a poor absorber in an a-Si:H solar cell of a thickness of about 300 nm. In the FDTD method we assumed periodic boundaries in the x and y direction and perfectly matched layers in the z direction. Optical properties of the materials were taken from literature.[14] Posterior to the FDTD simulation, the absorption was locally resolved by computing the divergence of the Poynting vector. The global absorption was subsequently obtained by integrating the local absorption over the a-Si:H layer. To study the impact of the intermediate layer, the global absorption for the stacks with intermediate layer were normalized with respect to results without the intermediate layer.

Figure 1(a) shows results for the absorption enhancement of the first scenario; only the intermediate reflector below the a-Si:H layer. Three essential observations can be made.

A decrease of the absorption in the presence of the intermediate reflector is found for $\lambda=658$ nm for all thicknesses. For 780 nm a very small increase is observed for small thicknesses. This is not surprising as the refractive index of the intermediate reflector is between the index of air and a-Si:H. The intermediate reflector in this configuration serves therefore as an antireflecting layer.

The second finding is the occurrence of a Fabry–Pérot-like oscillation, attributed to light that suffers from multiple reflections inside the intermediate reflector. The oscillation period can be deduced to be ≈ 250 and ≈ 200 nm for wavelengths $\lambda=780$ nm and $\lambda=658$ nm, respectively. This period deviates by a factor of 1.22 and 1.24 from the values observed in a flat thin film. The effect is attributed to the presence of the randomly textured interface causing an angular distribution of light inside the cell.[15] For inclined propagation directions, only the magnitude of the z component of the wave vector is of importance in setting the resonance condition for the Fabry–Pérot oscillation. However, this component is smaller when compared to light that propagates at normal incidence through the layer. Accordingly, scattered light in the solar cell can be understood as having an enhanced effective wavelength, causing the appearance of larger Fabry–Pérot periods. A pure geometrical picture will lead to an increased light path due to scattering and the wrong conclusion to need thinner layers for the same effect. Therefore, the wave nature of light cannot be neglected when designing intermediate layers for rough surface profiles. It is extremely complex to elucidate the effect quantitatively as the angular spectrum of the scattered field is difficult to resolve within a rigorous solution of Maxwell's equations. The only thing observable, which is the result of an exact simulation, is an effective Fabry–Pérot oscillation period from which one can extract an effective inclination angle inside the intermediate layer of 35°. This angle is not equivalent to the outer scattering angle, which can be measured by far-field optical experiments. The increase of the Fabry–Pérot period due to the textured surface is one important effect that has to be taken into account when designing intermediate reflectors. This increase might depend on the wavelength since the scattering properties of randomly textured surfaces are dispersive.

The third observation in Fig. 1(a) is a reduced oscillation amplitude for an increased thickness of the intermediate layer. The scattering process at the randomly textured interface leads to distributed out-of-plane components of the wave vectors. Consequently, the distribution function of the collected phase upon transfer through the intermediate reflector broadens with increasing thickness and interference effects become weaker. The absorption converges to an average value of the Fabry–Pérot oscillation.

This first scenario is not very close to a real device but it permits a clear distinction and identifications of all physical effects appearing in such systems. To match the analyzed system closer to a real-world device, Fig. 1(b) shows the absorption enhancement in the a-Si:H layer if an additional μc-Si:H layer with a thickness of 40 nm is sandwiched between the intermediate reflector and air. Again, a Fabry–Pérot-like oscillation with decreasing amplitude for increasing thickness can be observed. Instead of a reduced absorption compared to the system without intermediate reflector, an enhanced absorption was found, which is exclusively attributed to an increase of the Fresnel reflection in the stratified media below the a-Si:H layer.

Figure 1(c) shows the results of the third scenario, where the μc-Si:H was sufficiently thick to exclude any back reflection. This scenario comes closest to a real-world device and thus has the most practical relevance. A strong increase

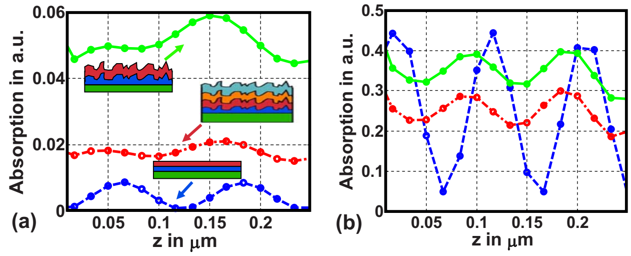

FIG. 2. (Color online) Depth resolved absorption profile in the a-Si:H layer for various solar cell structures. Blue dashed line denotes scenario (i) (flat interfaces and 250 nm a-Si:H on ZnO), green solid line denotes scenario (II) (randomly textured interfaces and 250 nm a-Si:H on ZnO), and the red dash-dotted line denotes scenario (III) (randomly textured interfaces and 250 nm a-Si:H on ZnO and μc-Si:H as the material in the transmissive half space). (a) $\lambda = 780$ nm and $h_{IL} = 150$ nm. (b) $\lambda = 658$ nm and $h_{IL} = 100$ nm. The depth resolved absorption is integrated over the x-y cross section.

of the absorption due to the presence of the intermediate reflector was observed with enhancement factors of up to 3 for a particular wavelength. The magnitude of the enhancement is larger than before. The increase derives at first from the increased index contrast at the back side of the top cell. Consequently, the two following mechanisms arise. (I) Due to the increased Fresnel reflection coefficient, the a-Si:H top cell acts like a thin-film cavity where field enhancement occurs. (II) The scattering strength is increased and the coupling efficiency to trapped light modes is larger compared to a system with only one scattering interface. The absorption enhancement for the longer wavelength of 780 nm is stronger compared to the shorter wavelength of 658 nm due to the larger intrinsic absorption coefficient of a-Si:H for 658 nm. Photon management is particularly important in the spectral domain of weak absorption in the a-Si:H layer.

Additionally to the global absorption enhancement, spatially resolved (along the z coordinate) absorption profiles inside the a-Si:H layer were evaluated by integrating the local absorption over the x-y plane. These profiles are shown for three selected scenarios and both relevant wavelengths in Fig. 2. For all three scenarios a ZnO layer is sandwiched between a glass substrate and a 250 nm a-Si:H layer where in (I) the ZnO layer is flat, but exhibits in (II) a randomly textured surface profile and (III) differs from (II) in that both an intermediate reflector and an infinitely thick μc-Si:H succeed the a-Si:H layer. The intermediate reflector had a thickness of 150 and 100 nm at the wavelength of 780 and 658 nm, respectively, which correspond to the maxima in Fig. 1(c). Two important findings can be noticed. First, in the spectral domain of weak absorption (780 nm), the randomly textured surface causes an enhancement of the absorption by a factor of about 8 where in the strong absorption domain (658 nm) this enhancement reduces to a factor of 2. The second important result is the strong homogenization of the absorption profile along the z coordinate although a minor modulation persists. This is directly correlated with the reduced Fabry–Pérot oscillation amplitude discussed in Fig. 1 and results also from the broadening of spectrum of spatial frequencies induced by the randomly textured interface. This absorption homogenization caused by randomly textured surfaces was already predicted in an early paper by Yablonovitch.[2]

In conclusion, the impact of an intermediate reflector layer integrated into an a-Si:H/μc-Si:H tandem solar cell on the absorption in the a-Si:H top cell was evaluated on the basis of exact numerical solution of Maxwell's equations. It was shown that the arising Fabry–Pérot oscillations have larger periods for randomly textured interfaces compared to flat interfaces. This shows that geometrical optics must not be used for designing these intermediate layers provided that rough interfaces are present. Moreover, the spectrum of spatial frequencies was broadened by the randomly textured interfaces, which damped the oscillations in the absorption enhancement for larger thicknesses of the intermediate reflector. Both results are extremely important for the design of intermediate reflectors for tandem solar cells as their effectively encountered properties are modified by these randomly textured surfaces. The results allow to predict optimized thicknesses of the intermediate reflector for a given wavelength regime.

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