Intermediate reflectors for enhanced top cell performance in photovoltaic thin-film tandem cells

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Abstract: We have investigated the impact of three types of intermediate reflectors on the absorption enhancement in the top cell of micromorph tandem solar cells using rigorous diffraction theory. As intermediate reflectors we consider homogenous dielectric thin-films and 1D and 3D photonic crystals. Besides the expected absorption enhancements in cases where photonic band gaps are matched to the absorption edge of the semiconductor, our results distinguish between the impact of zero order Bragg-resonances and diffraction-based enhancement at larger lattice constants of the 3D photonic crystal. Our full-spectrum analysis permits for a quantitative prediction of the photovoltaic conversion efficiency increase of the a-Si:H top cell.

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1. Introduction

The micromorph solar cell which we analyze in the present work consists of two different absorbing layers: amorphous silicon (a-Si:H) is the top and microcrystalline silicon (μc-Si) is the bottom cell [1]. Thus it is classified as a photovoltaic tandem cell. Generally, when compared to single absorber solar cells, the advantage of multi-junction cells (tandems) is their reduction of thermalisation losses and the possibility to absorb light oscillating at sub band-gap frequencies [2]. To put them in the context of nowadays research on solar cells, one may state that they belong to the so called 3rd generation solar cells [3]. They allow to obtain efficiencies close to or prospective even above those for single-junction solar cells. The efficiency of such single-junction solar cells is limited to approximately 28%, though their fabrication expenses are usually high. Since historically such single-junction solar cells were proposed first, they are usually called the 1st generation cells. But the micromorph tandem cell is also a thin-film cell: the thickness of the combined absorber layers is in the order of only a few microns and even smaller. Such thin-film solar cells belong to the 2nd generation solar cells. Their characteristic is a lower efficiency when compared to 1st generation solar cell but they can be fabricated at much lower costs; a property which renders them to be appealing for mass fabrication. In this context, the micromorph solar cell belongs to the 3rd generation since its evolution combines the advantages of both aforementioned generations. They constitute, generally, high efficiency solar cells which can be fabricated at reasonable low costs.

The combination of a-Si:H and μc-Si is particularly well suited for the concept since the different energetic positions of the absorption edges of a-Si:H (1.7 eV) and μc-Si (1.1 eV) allow to obtain high efficiency solar cells [4]. The a-Si:H top cell absorbs for this purpose high energy photons and delivers high voltage (0.9 V). Subsequent to the top cell, the μc-Si cell absorbs the transmitted low energy photons and delivers a lower voltage (0.35 V). In consequence of the direct electrical series-connection of both cells these voltages add. But series-connected

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tandem cells also have to be current-matched. Otherwise, the smaller current from one of the two cells will limit the current of the entire tandem. This is typically circumvent via tailoring the thicknesses of each cell to match their photocurrents. A reasonable thickness of a-Si:H however, is restricted to few hundred nanometers due to the small diffusion length of the holes, leaving a certain current mismatch ($j_{\mathrm{a-Si:H}} \neq j_{\mu\mathrm{c-Si}}$). The absorbance in the μc-Si cell in contrast can be increased by choosing a higher thickness. So, the first goal towards an improved performance of the tandem cell is the enhancement of absorption in the a-Si:H top cell. Therefore, this paper treats predominantly the a-Si:H top cell. We show in selected simulations that the thickness of the bottom cell can be fine tuned afterwards to determine the appropriate bottom cell that allows for the desired current matching.

Different optical devices in between both absorber layers can be used to force a redistribution of the photon flux in order to increase the top cell current. Photon management must be applied predominantly at frequencies of the a-Si:H absorption edge, as photons with significantly higher energies are fully absorbed even by thin a-Si:H cells, whereas photons with significantly lower energies are not absorbed at all.

Optical filters as intermediate reflecting layers (IRL) between the top and the bottom cell can assist for this purpose. IRL have successfully shown to increase absorption in top cells and thus the tandem efficiency [5]. Recently, micromorph modules of 13.4 % efficiency have been reported [6]. They make use of homogenous low-index intermediate TCO layers, while submodules without IRL are listed with 11.7 % efficiency, as certified by AIST [7]. Theoretical investigations of such layers reveal great potential of top cell current enhancement of about 25 % at the cost of a strongly reduced bottom cell illumination [8]. Preliminary experimental realization of (inverted) opal-based 3D photonic crystals (PhC) as IRL and their integration into tandem cells has already been reported [9], also addressing the important long-wavelength transmittance of the 3D PhC IRL. Photonic crystals in general are extremely appealing for an incorporation into solar cells [10]. The combination of strong reflectivity over a narrow spectral domain combined with diffractive effects due to the periodic interface stipulated a considerable wealth of research interest in the past [11, 12]. In most cases they found application as back reflectors [13]. The diffractive effect causes a prolongation of the optical path and enhanced so the number of absorbed photons [14]. Moreover, it permits to excite guided modes which allow to enhance absorption tremendously over a narrow spectral domain. If the solar cell is sufficiently thick the number of guided modes is likewise large and their excitation causes a strong absorption enhancement integrated over the spectral domain of interest [15].

In the present contribution we aim at elucidating the impact of various approaches for IRL on the absorption enhancement in the top cell of a tandem cell with rigorous diffraction theory. For this purpose we evaluate the spectrally dependent absorbance, based on material data of a-Si:H, as deposited for thin-film solar cells. This permits ultimately for an estimation of the enhancement of the number of absorbed photons when compared to the tandem cell without IRL. The three IRL under consideration have an increasing optical functionality. A homogenous dielectric film serves at first to increase the Fresnel reflection at the interface between both junctions. A Bragg stack comprising two media with different refractive indices serves at second to provide also a photonic band gap, causing a near-perfect reflection over a narrow spectral domain. Last, an inverted opal is considered, that provides in addition to the two aforementioned properties also a diffractive component. The combination of all three effects promises the strongest enhancement in the top cell. We present here a quantization of this enhancement for the three IRL on a-Si:H thin-film top cells.

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2. Numerical approach

To evaluate the absorption, we employ the Fourier Modal Method (FMM). It is a numerical technique that solves Maxwell's equations rigorously for periodic structures [16]. Close to a real device, the top and the bottom cells are assumed to be made of 0.2 μm a-Si:H:H and 1.5 μm μc-Si, respectively. Material parameters were taken from literature [17]. It is important to note that such interfaces will promote the amplitudes of thin-film oscillations significantly beyond those on their occurrence at imperfect real interfaces. But, in numerical simulation perfect interfaces ensure the comparability of interference-based IRL devices with different structural sizes and allow for a much more time-efficient calculation, thus increasing the achievable accuracy. Representative refractive indices were assumed for dielectric materials, e.g. polycrystalline ZnO (n = 1.7), monocrystalline ZnO (n = 2), or ITO (n = 2.5). The absorption is obtained by solving at first at each wavelength the diffraction problem using the FMM. Integrating the divergence of the Poynting vector **S** over the spatial domain occupied by the a-Si:H or the μc-Si layer provides the relevant locally resolved absorption. Weighting this absorption with the number of photons as provided by AM1.5 solar spectrum and a subsequent integration permits for computing the total number of absorbed photons. All simulations were normalized against the number of absorbed photons in the same tandem cell without the IRL. To evaluate the impact of the IRL design, a single characteristic design parameter was modified in each scenario.

The characteristic parameter for the homogenous dielectric IRL is its geometrical thickness $h_{\text{intermediate}}$. The refractive index of the homogenous dielectric layer was assumed to be 2.5; being the index of ITO. The characteristic parameter for the Bragg-stack is the optical thickness $h_{\text{opt}} = n_1 \cdot d_1 = n_2 \cdot d_2$ of both constituents. They have refractive indices of $n_1 = 1.7$ and $n_2 = 2.0$, respectively. The Bragg-stack consists of 10 unit cells, each comprising two material layers. The inverted opal consists of six layers of air spheres embedded in ITO. The characteristic parameter of the opal is the sphere radius R. The choice of materials orients on available materials for the fabrication.

3. Homogeneous IRL

Upon evaluating the **homogenous dielectric IRL**, Fig. 1(a) shows the absorption in the a-Si:H cell depending on the IRL thickness $h_{\text{intermediate}}$ and the wavelength λ. Modifying the thickness induces foremost Fabry-Pérot oscillations (FPO) in the reflectance spectrum. In passing we note that not only reflectance on its own causes increased absorption, but also the spectral position of a possible reflection peak relative to the absorption edge affects the efficiency. Matching both features leads to optimal absorption enhancement.

The IRL shows no effect on the absorption at short wavelengths. In this spectral domain, a-Si:H is sufficiently absorptive and a single passage of photons through the layer is sufficient to ensure their complete absorption. Above 550 nm oscillations in the absorption are observed, being reminiscent to the aforementioned FPOs. Naturally, with increasing thickness of the IRL their period tends to be smaller in the spectral domain. Above approximately 700 nm, the absorptive properties of the a-Si:H are almost negligible and the IRL has no influence.

The enhancement of the number of absorbed photons integrated over the entire spectrum is shown in Fig. 1(b). An absolute maximum occurs for a IRL thickness of about 60 nm, where a reflection maximum matches the absorption edge of a-Si:H. As a function of the IRL thickness the number of absorbed photons shows similar FPOs, though the envelope of the oscillations decreases for thicker layers towards a mean value that would appear for incoherent light. This mean value of absorption enhancement is approximately 4%. The enhancement factor is a consequence of the refractive index contrast at the interface from the high-index top cell to the low-index IRL. An interface between non-absorbing media ($n_1 = 3.6, n_2 = 2.5$) would yield 3.25 % of Fresnel reflectance. A stronger index contrast would naturally increase the absorption

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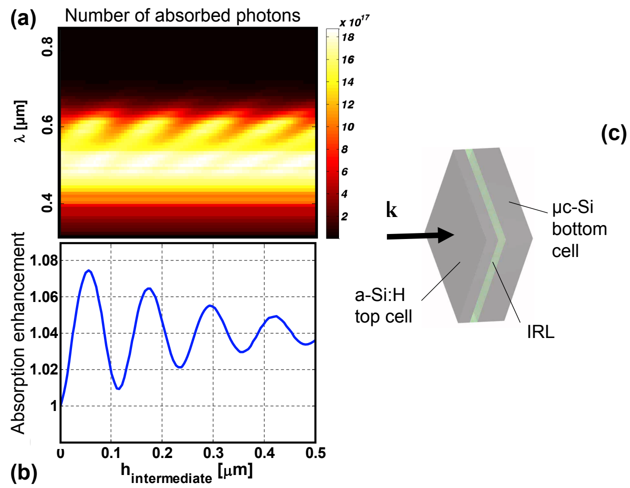

Fig. 1. The number of absorbed photons weighted with the solar spectrum in a-Si:H as a function of the wavelength and h_{im} is shown in (a). The enhancement of the number of absorbed photons as a function of $h_{intermediate}$ for the homogenous dielectric IRL is shown in (b), while (c) shows a scheme of the model geometry.

enhancement.

4. 1D photonic crystals

The **Bragg-stack** is understood here as a prototypical example for a one dimensional photonic crystal. Photonic crystals are characterized by a periodic modulation of the permittivity in space. Similar to a periodic potential in a solid state material and the introduction of a band structure for the electron wave functions, the periodicity of the PhC strongly affects the properties of light propagation. To describe from a theoretical point of view the light propagation in such photonic crystals, one usually relies on the application of Bloch's theorem and the so-called photonic master equations. They can be directly obtained from Maxwell's equations. They constitute wave equations that can be used to fully describe the light propagation in such periodic photonic materials. The master equations solve basically for the field distributions and the eigenfrequencies of the eigenmodes that are allowed to propagate in the photonic crystal. By computing the eigenfrequency in dependence on the wave vector that defines the principal propagation direction of the eigenmodes, a dispersion relation can be constructed. All information required to describe the light propagation in the bulk photonic crystals will be included in this dispersion relation. The dispersion relation in general is a versatile concept and finds use in optics whenever the object comprises a periodicity [20, 21]. A thorough discussion of the principles of 1D PhC can be found, e.g. in chapter 4 of Ref. 22. If for a given wave vector no solutions exist within a certain spectral domain, the propagation of light through the PhC is inhibited at these frequencies. In analogy to an electronic band structure one speaks of a photonic band gap; a spectral domain for which no propagating solutions exist but only evanescent. Illuminating a 1D PhC in this spectral domain causes strong reflectance over a spectrally narrow domain. If such a reflection gap is solely provoked by the periodic arrangement of the photonic material in space one usually speaks of a Bragg gap. The evaluation of the impact of such a Bragg gap for a 1D PhC on the top cell's absorption is presented in Fig. 2.

Similarly to the homogenous IRL, the Bragg-stack produces pronounced oscillations in the absorption spectrum as shown in Fig. 2(a). The oscillation periods are much smaller as the

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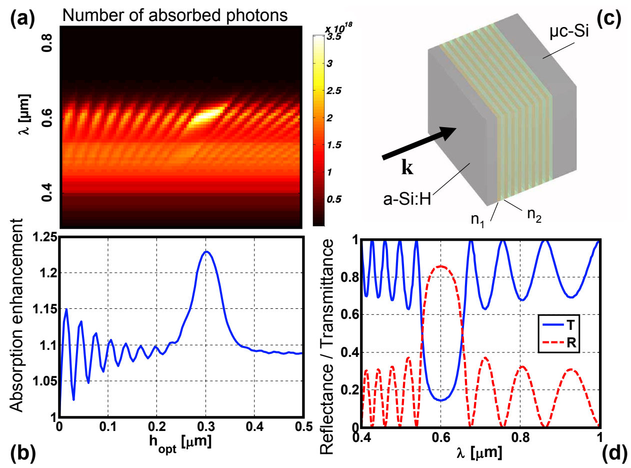

Fig. 2. (a) The number of absorbed photons in the a-Si:H cell weighted with the solar spectrum as a function of the wavelength and h_{opt} for a Bragg stack as IRL is shown in (a). The enhancement of the number of absorbed photons as a function of h_{opt} is shown in (b). (c) shows the geometric Bragg layer structure. The optical spectra of the Bragg stack where absorption enhancement has its maxima is shown in (d).

absolute thickness of the structure is larger. Furthermore, the maximum absorption is higher when compared to the homogenous IRL because the first layer of the stack was assumed to have a lower refractive index of $n_1 = 1.7$. The strong index contrast is beneficial for an increased Fresnel reflection. The enhancement of the number of absorbed photons as shown in Fig. 2(b) compares in nearly the entire spectral domain to the observations made for the homogenous IRL. The only deviation occurs if the spectral position of the photonic band gap of the Bragg stack compares to the spectral domain of the a-Si:H absorption edge; namely between 550 nm and 700 nm. A maximum of absorption enhancement occurs at $h_{\text{opt}} = 0.3\ \mu$m, as shown in Fig. 2 (b). The absorption enhancement is significantly elevated above the value that could be obtained at incoherent illumination and by employing a Fresnel reflection only, which would correspond to the mean value in the oscillating region.

The observed enhancement may be unambiguously attributed to the occurrence of the photonic band gap, a zero order Bragg resonance, in the proper spectral domain. This can be deduced from Fig. 2(d). The band gap is centered around 600 nm. By spectrally matching the photonic band gap with the absorption band edge, the absorption enhancement gets larger. This is exclusively attributed to the impact of photon management. Overall absorption is enhanced by a factor of 1.22 when compared to a solar cell without intermediate reflector.

At the example of this optimized IRL that causes the largest absorption enhancement in the top cell, we detail the impact of the IRL also on the bottom cell. In accordance to the introduction, we require that the bottom cell has to be current matched to the top cell. It implies that the same number of photons has to be absorbed. The number of absorbed photons in the top and the bottom cells depending on the thickness $h_{\mu\text{c}-\text{Si}}$ of the bottom cell are shown in Fig. 3 . The remaining parameters of the cell correspond to those for which the absorption enhancement as shown in Fig. 2(c) has its maximum. All the properties as outlined in the introduction can be revealed. The absorption in the top cell is not affected by the peculiar choice of the thickness of the μc-Si cell, though weak modulations can be seen. They occur if the thickness of the bottom cell is negligible and a noticeable share of light is suffering from multiple reflections. With increasing thickness of the bottom cell the number of absorbed photons in the bottom

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cell increases steadily as expected. Current matching is achieved for a μc-Si cell thickness of 1.55 μm. By further increasing the thickness of the bottom cell the absorption tends to saturate. But an increase of thickness beyond 1.55 μm would be pointless since the current of the solar cell would be limited by the current of the top cell. The same procedure to adjust the thickness of the bottom cell would apply for any other intermediate reflector.

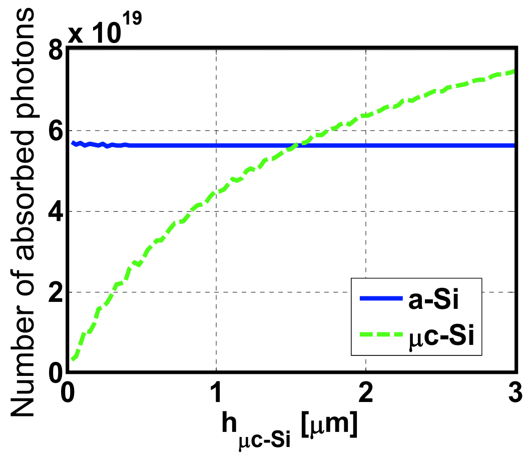

Fig. 3. Number of absorbed photons in the top and the bottom cell depending on the thickness of the bottom cell. The parameters of the Bragg-type IRL correspond to those for which absorption enhancement has its maximum [see Fig. 2(d)].

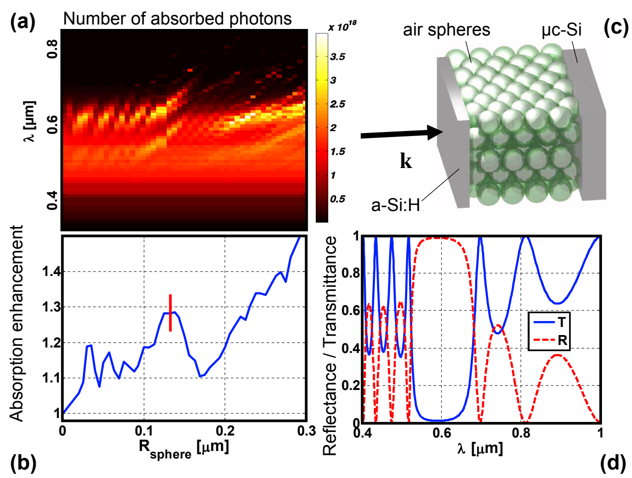

Fig. 4. (a) The number of absorbed photons in the a-Si:H cell weighted with the (AM1.5) solar spectrum is shown in (a) as a function of wavelength and sphere radius R for an inverted opal IRL. The enhancement of the number of absorbed photons as a function of R is shown in (b). (c) shows the schematic opaline IRL geometry. The optical spectra in (d) correspond to the sphere radius at the local maximum at R = 130nm in (b).

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5. 3D photonic crystal

If the high reflectance within the photonic band gap is combined with a diffracting structure a further significant enhancement in the number of absorbed photons can be observed. Results by using an **inverted opal** for this purpose as an IRL are shown in Fig. 4. The inverted opal consists of six layers of spheres.

With respect to both quantities, the spectral width and the magnitude, the 3D PhC has a stronger photonic band gap when compared to the Bragg stack. It is caused by a photonic stop-gap in ΓL-direction of the 3D fcc-lattice of the hard-sphere crystal [18]. Its spectral position depends on the sphere radius. For small spheres, this band gap occurs at small wavelengths where light management has no importance: a-Si:H is sufficiently absorptive. The details of the opal structure are not resolved by light oscillating at larger wavelengths. Light therefore merely experiences an effective index. Hence, for small sphere radii the absorption [Fig. 4(a)] and the absorption enhancement [Fig. 4(b)] show FPOs, comparable to the homogenous dielectric IRL. Increasing the radius allows to tune the photonic band gap to spectrally coincide with the absorption edge. Again, a strongly enhanced absorption enhancement occurs over a narrow spectral domain if both are matched. This occurs for a sphere radius of approximately 130 nm for the index contrast of air spheres (n = 1.0) embedded in ITO (n = 2.5) [18]. The optical spectrum of the corresponding opal is shown in Fig. 4(d). The overall enhancement of the number of absorbed photons for an optimized opal amounts then to a factor of 1.3 when compared to the cell without IRL. Besides this effect of zero order Bragg reflection of light, for larger radii the structure tends to diffract light into guided modes inside the a-Si:H layer. Upon excitation of such guided modes the path of the photons is enlarged and so is their probability to get absorbed. First, this causes a much stronger enhancement when using an opal as compared to a Bragg stack. And second, it causes most likely also the continuous increase of the diffraction-based enhancement of absorption at larger sphere radii. The larger the spheres the denser is the spectrum of possible guided eigenmodes excited. The necessary condition for their excitation is a match between the transverse momentum provided by the opaline grating and the propagation constant of a guided eigenmode. The excited eigenmodes can be clearly seen as sharp peaks in the absorption spectra in Fig. 4(a). An absorption enhancement up to a factor of 1.5 is feasible. The limits of the absorption enhancement by using much larger spheres were not evaluated and are currently under investigation.

6. Summary

In conclusion, we have analyzed the absorption enhancement in the top cell of a micromorph tandem solar cell upon incorporating various intermediate reflectors. It is shown that the integrated absorption enhancement can be significantly increased above the level achievable with a homogenous dielectric intermediate reflector. This can be achieved if a photonic crystal is created with a photonic band gap that spectrally matches the absorption edge of a-Si:H. Employing such a scenario, the enhancement of the number of absorbed photons reaches a factor of 1.3 when compared to a solar cell without intermediate reflector. This makes it a promising candidate for a practical solar cell device that employs novel concepts of photon management.

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