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Decoupled textures for broadband absorption enhancement beyond Lambertian light trapping limit in thin-film silicon-based solar cells

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Abstract — **We present a modelling study of thin silicon-based solar cells endowed with periodic and decoupled front/back textures. After careful optimization, the proposed device models exhibit absorption beyond the Lambertian light trapping limit for a wide range of light angles of incidence. The advanced light management scheme is applied to (nano)-crystalline silicon solar cells, where the benefits of texturing the absorber rather than the supporting layers is clear, and to barium (di)silicide solar cells, which could achieve an implied photocurrent density of 41.1 mA/cm2 for a thickness of only 2 µm.**

Index Terms — **barium silicide, Lambertian scattering, light trapping, nano-crystalline silicon, periodic gratings, thin-film silicon.**

I. INTRODUCTION

Solar cells with silicon absorber material currently dominate the photovoltaic (PV) market [1]. Next to record-efficiency wafer-based devices [2], thin-film silicon (TFSi) multi-junction architectures with hydrogenated nano-crystalline silicon (nc-Si:H) absorbers have achieved initial and stabilized conversion efficiencies up to 16.3% and 14%, respectively [3]-[4]. In spite of the lower performance, TFSi devices display the smallest cell-to-module losses of all thin-film technologies [5], and can thus still play a relevant role in the PV market. In addition, the relatively low absorption coefficient of (nano)-crystalline silicon makes it an ideal candidate for testing various light management approaches, e.g. random/periodic texturing, dielectric spacers and reflectors, metallic nano-particles, etc. [5]-[10].

In this contribution, we present an investigation of the optical performance of thin silicon-based solar cells, endowed with decoupled gratings at the front and at the back side of the device. We first study the case of nc-Si:H [11], where the periodic textures were directly applied to the absorber layer. After a thorough geometrical optimization of the top and bottom pyramidal gratings, an implied photocurrent density (J_{ph}) of 36 mA/cm^2 was achieved, for a device endowed with a 2-µm thick absorber. The obtained value is above the Lambertian light trapping limit, for an equally thick slab of nc-Si:H over the light spectrum between 300 nm and 1200 nm, for angles of incidence up to 60°.

Aware of the negative impact of textures on the surface recombination of charge carriers, we then compare the performance of the previously optimized gratings to a similarly textured but electrically flat structure, based on a crystalline-silicon (c-Si) absorber [12]. To simplify the analysis, only the case of perpendicular incidence of light was considered. A significant decrease of J_{ph} was observed, highlighting the need of good passivation to ensure an efficient charge collection, particularly in the presence of highly textured interfaces.

Finally, we apply the same light management approach to a novel and promising silicon-based alloy, barium (di)silicide ($\mathrm{BaSi_2}$) [13]. Thanks to the higher absorptivity of this material (with respect to nc-Si:H), a remarkable J_{ph} of 41.1 mA/cm^2 was obtained, for an absorber thickness of only 2 µm.

II. METHODS AND THEORETICAL FRAMEWORK

A. Optical simulations

The study here presented has been carried out via optical modelling, employing the High Frequency Structure Simulator (HFSS) provided by ANSYS. The software is a rigorous Maxwell equation solver, based on the finite element method [14].

Input information for the simulations are the device geometry and the carefully measured optical properties (refractive index and extinction coefficient) of state-of-the-art materials used in real devices [11]. The reflection (R) and the absorption in each layer of the solar cell models (A_i) are calculated and then convoluted with the photon flux of the standard AM1.5 spectrum ($\Phi_{\mathrm{AM1.5}}$) [15], to obtain the implied photocurrent density ($J_{\mathrm{ph}-i}$) generated (in the absorber) or lost (in supporting layers or due to reflection):

$$J_{\mathrm{ph}-i} = -q\int_{300\ \mathrm{nm}}^{1200\ \mathrm{nm}} A_i(\lambda)\Phi_{\mathrm{AM1.5}}(\lambda)\,d\lambda \qquad (1)$$

where q is the elemental charge and λ the wavelength of light. In the ideal case of perfect collection of photogenerated charge carriers, the J_{ph} calculated for the absorber layer would represent the short-circuit current density (J_{SC}) generated in an equivalent real device. Hence, the computed photocurrent density value can be considered the upper limit of J_{SC} that can be achieved.

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B. Performance analysis and optical limits

When analyzing the effectiveness of novel light management approaches, it is important to evaluate their performance in comparison to theoretically calculated absorption limits, and to quantify the achieved improvements with respect to the standard situation, usually a flat reference device.

The absorption of perpendicularly incident light by an uncoated flat slab of material – with absorption coefficient α and thickness d – is usually referred to as *single-pass* absorption (A_{SP}):

$$A_{SP} = 1 - e^{-\alpha d} \xrightarrow{\alpha d \ll 1} A_{SP} \approx \alpha d \qquad (2)$$

It can be observed that, in weak absorption conditions (αd << 1), A_{SP} can be approximated by the product of absorption coefficient and thickness. This αd term is used to determine the enhancement factor (*EF*), which is an indicator of how much absorption in a material (A) is improved with respect to the reference *single-pass* case:

$$EF = \frac{A}{A_{SP}} \approx \frac{A}{\alpha d} \qquad (3)$$

If a perfect mirror is placed at the back side of the layer, light can pass twice through the slab (*double-pass* absorption, A_{DP}):

$$A_{DP} = 1 - e^{-2\alpha d} \xrightarrow{\alpha d \ll 1} A_{SP} \approx 2\alpha d \qquad (4)$$

It is apparent that, in the limit case of weak absorption, A_{DP} is exactly double than the value of A_{SP}.

A material endowed with a perfect back reflector and an ideal Lambertian scatterer will enhance the *single-pass* absorption by the well-known $4n^2$ factor [16]-[17]:

$$A_{Lamb.} = \frac{1 - e^{-4\alpha d}}{1 - \left(1 - 1/n^2\right) e^{-4\alpha d}} \xrightarrow{\alpha d \ll 1} A_{Lamb.} \approx 4n^2 \alpha d \qquad (5)$$

where n is the refractive index of the material. Eq. (5) is also known as the *Yablonovitch limit*, although in specific conditions (e.g. with the use of periodic gratings and in a limited range of angles of incidence) such absorption "limit" can be surpassed – as shown by Yu *et al.* in their calculation of optical limits in grating structures using the Temporal Coupled-Mode theory [18]. Evidently, the *EF* in the Lambertian limit case is exactly equal to $4n^2$, which in the case of (nano)crystalline silicon corresponds to ~ 50 in the spectral region near the material bandgap (~ 1100 nm). All the results of the simulations of this work are compared with the three aforementioned limits (*single-pass*, *double-pass* and *Yablonovitch*), to assess their optical performance.

III. RESULTS AND DISCUSSION

We first look into the case of nc-Si:H thin-film devices. The thickness of the absorber (2 μm) and of the supporting layers are summarized in Fig. 1. The top and bottom pyramidal textures were geometrically optimized to maximize the implied J_{ph}. An extensive set of base and height values was tested, for both front- and back-side pyramids. Ultimately, the best structure is endowed with pyramids at the top with both base (b) and height (h) equal to 700 nm. The high aspect ratio of the features (AR = h/b = 1) results in excellent light in-coupling, as shown in Fig. 2 by the very low reflectance at wavelengths between 300 nm and 900 nm (at longer wavelengths secondary reflectance from the back side starts to appear). At the rear, the optimal configuration consists of pyramids with base and height of 1200 nm and 300 nm, respectively. In this case a lower aspect ratio (AR = 0.25) is preferred, to reduce the amount of light absorbed by the back contact, while maintaining an efficient scattering on near-infrared photons that reach the textured reflector.

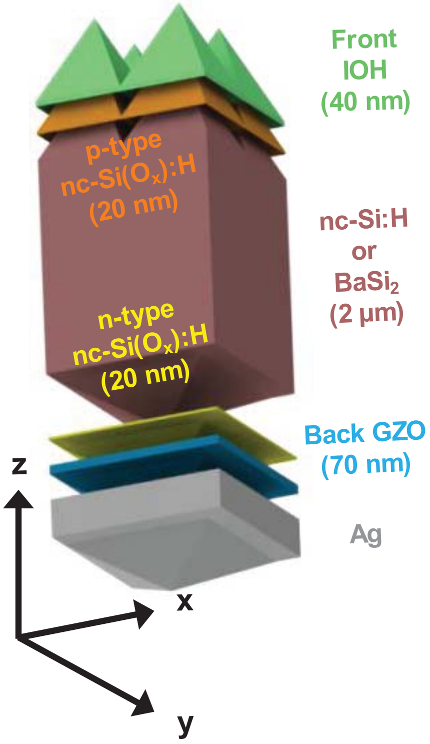

Fig. 1. Modelled solar cell structure based on nc-Si:H or BaSi$_2$.

The period (P) of the combined front/back decoupled texture is set to twice the value of the top pyramid base (i.e. P = 1400 nm), allowing the bottom texture to by asymmetrically positioned with respect to the top (see Fig. 1). The breaking of the symmetry promoted better light trapping, resulting in an implied J_{ph} of 36.0 mA/cm^2 for perpendicular incidence of light. This value is higher than the one calculated by convoluting the Lambertian limit absorption ($A_{Lamb.}$) with

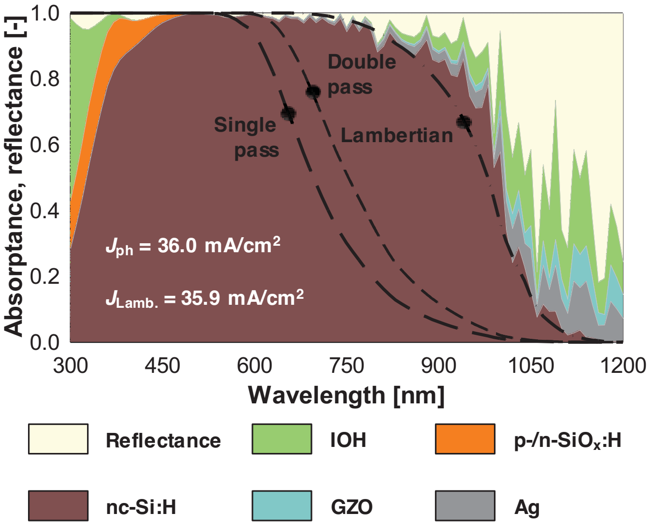

Fig. 2. Reflectance and absorptance of all layers of the nc-Si:H solar cells model. The implied photocurrent density of the absorber (36.0 mA/cm^2) is higher than that of the Lambertian limit of an equivalently thick nc-Si:H (35.9 mA/cm^2).

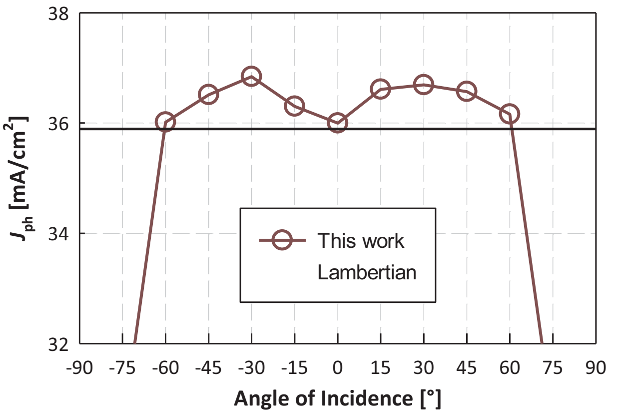

Fig. 3. Photocurrent density in the nc-Si:H layer of the structure of Fig. 1 (brown line), for angles of incidence from –90° to 90°. The black line indicates the value in Lambertian limit conditions

$\Phi_{AM1.5}$ ($J_{Lamb.}$ = 35.9 mA/cm^2), despite the presence of (parasitically) absorbing supporting layers such as the front transparent contact and the p- and n-type doped layers. Such remarkable performance is evidenced by the absorption spectrum of nc-Si:H (see Fig. 2, in brown), which in the near infrared region is regularly above the *Yablonovitch limit*. The remarkable performance can be mainly attributed to the concurrent excitation – by both front and back gratings – of guided mode resonances inside the absorber [11].

Within the weak absorption region (1000 nm < λ < 1200 nm), the average value of the enhancement factor for our proposed device architecture is $EF_{\text{nc-Si:H}}$ = 63.9, significantly higher than the value than could be achieved in Lambertian limit conditions ($EF_{\text{Lamb.}}$ = 50.4). Moreover, the obtained value is also higher than the one calculated for an equivalently thick layer of nc-Si:H endowed with a grating with P = 1400 nm (EF_{grating} = 51.1) [11], with the help of the temporal coupled-mode theory as developed by Yu *et al.* [18]. This result highlights the need for an extension of the current theory, to include advanced approaches such as the one proposed in this contribution.

The final point of interest – when investigating the optical performance of solar cells – is to study their angular sensitivity, i.e. how the absorption in the active layer of the structure changes for different direction of incident light. For the structure of Fig. 1, several values between 0° and 90° were tested, in both the positive and negative direction along the x-axis. Results (see Fig. 3), expressed with respect to the J_{ph} value of the Lambertian limit (35.9 mA/cm^2), show that the response of the solar cell model is non-symmetric, as expected, and that an optical performance equal or superior to the *Yablonovitch limit* case is achieved for angles of incidence up to 60°, and only decays (albeit sharply) for larger angles.

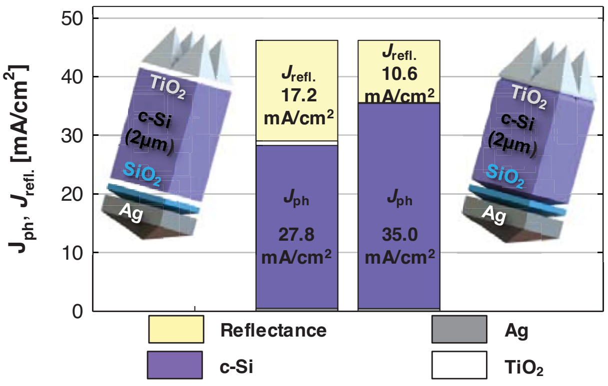

Fig. 4. Implied photocurrent density generated (in c-Si) and lost (in supporting layers, or due to reflection), for models with textured dielectrics (left) or textured silicon (right).

The proposed nc-Si:H solar cell structure performs very well optically, achieving high implied photocurrent density values (36 mA/cm^2) in a very thin absorber (2 μm). However, the textured interface between absorber and contacts could lead to significant recombination of charge carriers, thus greatly decreasing the final device efficiency. Therefore, we investigated the impact of texturing the supporting (dielectric) layers rather than the (nano)crystalline silicon absorber. This study was carried out for 2-μm thick c-Si layers, coated with a TiO$_2$ layer on the top, and a SiO$_2$/Ag bottom mirror. While this structure resembles a full device, we would like to stress that it is not the depiction of a complete solar cell, since the selective contacts are missing (see inset in Fig. 4). The front/back decoupled pyramidal texture has similar dimensions as the one optimized in the previous section of the manuscript for nc-Si:H, the only difference being the period (set to 1200 nm in this case). In fact, the base of front pyramids is set to 600 nm, while the height was kept at 700 nm.

Results of the simulations (see Fig. 4) show that the model with pyramids embedded directly on the silicon layer (J_{ph} = 35.0 mA/cm^2) performed significantly better than the one where the dielectric layers are textured (J_{ph} = 27.8 mA/cm^2). However, the latter configuration will likely yield higher voltage and fill factor, thanks to the flat silicon-dielectric interfaces. Nevertheless, these results highlight the importance of having high-quality surface passivation in c-Si devices, to allow an efficient charge collection even in the presence of significantly textured interfaces, such as the one proposed in this work.

Finally, our advanced light trapping scheme was applied to a novel and promising material, $BaSi_2$. This silicon alloy displays very favorable opto-electrical properties, such as long carrier diffusion length (~10 µm), a quasi-direct bandgap of 1.25 eV, and a high absorption coefficient [13],[19]. The proposed device structure closely resembles that of single-junction TFSi devices, where the nc-Si:H absorber is replaced by $BaSi_2$ (see Fig. 1).

Results in Fig. 5 show once again that the computed absorption – in the case of perpendicular incidence – can surpass the Lambertian limit, albeit in narrower region than in the nc-Si:H case, owing to the higher absorptivity of $BaSi_2$. Nevertheless, an implied J_{ph} of 41.1 mA/cm^2 is achieved for a device with an absorber thickness of only 2 µm, displaying the great potential of $BaSi_2$ as novel absorber for thin-film solar cells.

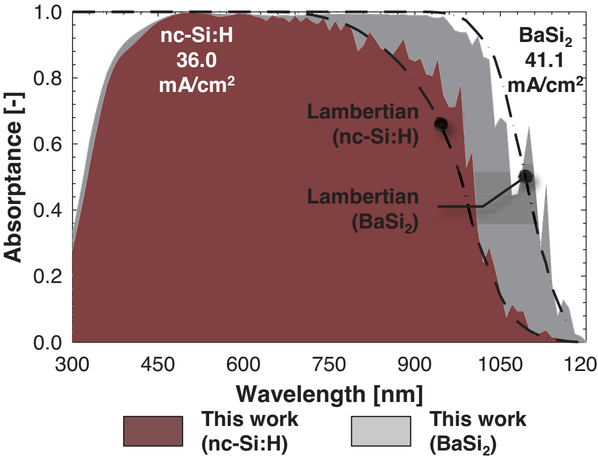

Fig. 5. Absorption spectrum of solar cell models with nc-Si:H (brown) and $BaSi_2$ absorbers (gray), embedded with an optimized decoupled front/back pyramidal texture.

IV. CONCLUSIONS

We presented an advanced light management approach, consisting of decoupled front/back periodic pyramidal textures applied to silicon-based thin-film solar cells. Thanks to the presence of gratings at the top and at the bottom side, the Lambertian light trapping limit was surpassed in a wide range of wavelengths, and for a wide range of angles of incidence. We further showed how texturing the active (silicon) layer yields significantly better results than embedding the gratings in the supporting (dielectric) layers, stressing the need of high-quality passivation of the absorber to effectively collect the photogenerated charge carriers. Finally, the great potential of novel absorber $BaSi_2$ is displayed, for which an implied photocurrent density of 41.1 mA/cm^2 is achieved for an absorber thickness of only 2 µm.

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