Infrared Absorption Enhancement Using Periodic Inverse Nanopyramids in Crystalline-Silicon Bottom Cells for Application in Tandem Devices

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Abstract—Carefully tailored periodic nanostructures on the light wavelength scale, such as diffraction gratings, benefit from wave optics for efficiently trapping the weakly absorbing infrared photons in crystalline-silicon (c-Si) absorbers. In contrast with the conventional random pyramid texture, diffraction gratings can be designed to target specific wavelength ranges by the selection of the grating pitch. Absorption enhancement at infrared wavelengths in a silicon solar cell is especially desired when it operates below a perovskite top cell in a tandem device. In this article, inverse nanopyramid gratings of 800 nm pitch are proposed as an alternative front-surface texture to random pyramids in silicon heterojunction devices with interdigitated back contacts that are to be used as bottom cells in four-terminal perovskite/c-Si tandem devices. By doing so, we report a short-circuit current density gain of 0.53 mA/cm² with respect to the random pyramid texturing for the bottom c-Si cell. The rationale to substitute random pyramids by inverse nanopyramid gratings is, however, not justified in single-junction operation despite achieving the power conversion efficiency of 22.3% since the degraded optical performance at shorter wavelengths offsets the absorption enhancement at longer wavelengths, resulting in similar levels of short-circuit current densities for both texture types.

Index Terms—Heterojunction, interdigitated and back contact (IBC), light trapping, nanoimprint lithography (NIL), nanophotonics, solar cells, tandem cells.

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I. INTRODUCTION

SIGNIFICANT advancement in the silicon photovoltaics (PV) technology over the past decades has drastically reduced the price of silicon solar cells and modules. With solar panels becoming increasingly more affordable, further reduction in the levelized cost of electricity is predominantly now constrained by the area-dependent installation expenses [1]. Examples of these expenses, labeled as the balance-of-system costs, include the cost of wiring, mounting structures, inverters, batteries, and other components constituting a PV system. Since the balance-of-system costs scale-up with the area, they can potentially be lowered by raising the cell and module-level power conversion efficiencies (PCEs) so that more power can be generated per unit area.

Crystalline-silicon (c-Si) solar cells have already attained remarkable conversion efficiencies beyond 26% [2]–[4], thereby closing the gap with the intrinsic limit of 29.4% [5]. However, the practical limit for c-Si cells is estimated to be only around 27% once the resistive losses are taken into consideration [3]. Therefore, room for further efficiency improvement with single-junction (S-J) c-Si cells is marginal and calls for the application of more sophisticated cell concepts to surpass the fundamental S-J c-Si efficiency barrier [6]. One of the reasons for the relatively low fundamental efficiency limit of c-Si cells is the nonoptimal utilization of excess photon energy. Being referred to as thermalization losses, the extra energy of ultraviolet wavelength photons above the bandgap of c-Si is wasted as the photogenerated carriers relax to the conduction and valence band edges by emitting phonons. Mitigating thermalization losses is possible, for instance, by employing the multijunction approach in which several absorber materials of complementary bandgaps are stacked on top of one another such that the higher energy photons are absorbed in wider bandgap materials, while the narrower bandgap absorbers only receive the lesser energy photons. This way, the total efficiency can be raised above that of individual subcells that make up the multijunction cell structure. Since most progress in PV research for terrestrial applications is driven by cost-savings, the double junction or the tandem configuration represents the simplest and most cost-effective multijunction cell structure with the potential of reaching PCE values as high as 46% [7] under the standard AM 1.5G solar spectrum and intensity.

In combination with a c-Si bottom cell, organic–inorganic hybrid perovskites have emerged in recent years as promising top-cell candidates for tandem devices [7]–[15]. Besides, the low processing cost of perovskites using solution-based [16], [17] or vapor deposition [18] methods, perovskites exhibit a steep absorption edge [19] and their bandgap can be tuned over a wide range [20], [22], making them attractive top-cell absorbers. Perovskite/c-Si tandem devices are normally realized in two-terminal (2-T) and four-terminal (4-T) configurations with each design offering certain advantages over the other. The 2-T design involves the deposition of perovskite cell layers on an underlying c-Si cell so that both subcells are electrically connected in series. The 2-T design is attractive since additional circuitry at the system level is not required while keeping the parasitic absorption losses minimal by only utilizing a single transparent electrode. However, the current-matching requirement of the configuration [23] demands tight control over the bandgap and the thickness of the top-cell absorber layer. Another challenge with the 2-T design is to conformally deposit the perovskite cell layers on a textured c-Si bottom cell without damaging the functional layers underneath [24]. On the other hand, in the 4-T case, individual subcells can be optimized and fabricated separately and later coupled optically by mechanical stacking. The configuration, therefore, offers more freedom in the choice of bottom c-Si cell architecture, specifically now tailored to operate under the infrared (IR) part of the AM 1.5G spectrum. Perhaps the biggest advantage of the 4-T configuration over its 2-T rival is the absence of current-matching requirement between the subcells. It implies that a 4-T device efficiency is less sensitive to spectral composition variations, translating into a higher annual energy yield [66], [67], to compensate for the additional circuitry cost at the system level.

In order to maximize the open-circuit voltage (V_{OC}) of the narrower bandgap c-Si subcell, cell technologies incorporating passivating contacts [25], [26] could be used to reach the unprecedented levels of V_{OC} by significantly curtailing carrier recombination losses at the contacts [27]–[32]. Amongst the numerous materials reported to implement passivating contacts, the highest voltages to date for S-J c-Si cells were achieved by deploying hydrogenated amorphous silicon (a-Si:H) thin-film stacks [33], [34]. In this silicon heterojunction (SHJ) cell technology, excellent surface passivation is enabled by depositing intrinsic and *in situ* doped a-Si:H thin-film stacks that saturate the dangling bonds at the surfaces and provide band bending at the c-Si surface for the carrier selectivity [35], [36]. Moreover, it is also possible to eliminate grid-shading losses by implementing both terminals of the device on the rear side in an interdigitated and back-contacted (IBC) cell structure [37]. The merger of SHJ and IBC cell concepts, i.e., SHJ-IBC, led to the record 26.7% cell efficiency for S-J c-Si devices [2]. From the perspective of 4-T tandem devices, the SHJ-IBC architecture is particularly well suited for bottom-cell usage as both contacts are situated on the rear side, which reduces the number of required transparent electrodes by one. Another optical advantage of the structure is that the passivating a-Si:H stacks are transparent to the incoming IR photons, thereby allowing the adaptation of their thickness for optimal electrical performance without contributing to

additional parasitic absorption losses. Unlike diffused junction cells, free-carrier absorption losses are also minimized in this cell structure. Finally, the SHJ-IBC architecture can be used in conjunction with the advanced light management strategies to boost the IR absorption in these devices.

Advanced light management strategies nowadays include substituting the industry-standard random pyramid (RP) texture by diffraction gratings [38]–[46], [58], black-silicon [47]–[49], or other nanoscale textures [50]–[56] in solar devices. Amongst many nanoscale texturing alternatives, periodic wavelength-scale textures, such as gratings, profit from diffraction to enhance absorption at wavelengths corresponding to the grating pitch [43], [57]. In the case of RP texture, trapping efficiency of in-coupled photons within the absorber is dependent on the incidence angle as described by geometrical optics. However, this angular dependence can be circumvented by trapping light instead of in the wave optics regime. For the wave-optical case, superior optical performance with respect to RP texture at desired wavelengths is attributed to the excitation of waveguide modes in the photoactive layer, which are controlled by the grating pitch [59]. The introduction of diffraction gratings on the rear side of the c-Si bottom cell in a 2-T GaInP/GaAs/c-Si triple-junction device led to an impressive 33.3% PCE [60]. This work by Cariou *et al.* [60] demonstrates a short-circuit current density (J_{SC}) gain in the c-Si subcell of 1.1 mA/cm² compared with the flat reference. In a 4-T configuration, where there are no constraints on the geometry of the front-side texture, it remains to be ascertained if the presence of diffraction gratings on the front side of a c-Si bottom cell is optically more favorable than its RP-textured analog, which is the main goal of this article.

In this article, we propose the integration of inverse nanopyramid (INP) gratings as the front-surface texture in SHJ-IBC cell structure for application in 4-T perovskite/c-Si tandem devices. We demonstrate increased IR absorption in c-Si devices by front-side nanopatterning as opposed to the standard RP texturing, thus providing an additional route to enable higher bottom-cell efficiencies.

II. EXPERIMENTAL DETAILS

A. Nanoimprint lithography (NIL) Process

SiO_x was deposited by plasma-enhanced chemical vapor deposition (PECVD) at 225 °C on both sides of the c-Si substrate (*n*-type float zone, 200 μm thick, and 3.0 Ω·cm base resistivity) to serve as metal-contamination protection on the rear and lithography mask on the front. Resist (mr-I 7010R from microresist technology) was then spun on to the side to be patterned. Spin coating was followed by pattern transfer from the soft stamp (silicone elastomer Sylgard 184 from Dow) to the resist by thermal imprinting in a hydraulic press at 130 °C. Next, SiO_x on the front side was patterned by consecutive O₂ and CF₄ reactive ion etching (RIE) steps. The INP pattern was formed by wet chemical anisotropic etching in TMAH: H₂O = 2: 3 solution with a commercial surfactant at 80 ± 2 °C. In the last step, SiO_x was removed by a short dip in HF: HCl: H₂O = 1: 1: 20 solution. The NIL process is depicted in Appendix A

and reported in detail in previous works with adaptation in RIE steps [44], [45].

B. Random Pyramid (RP) Texturing

Reference single-side RP-textured samples were prepared by protecting one side by depositing PECVD $\text{SiO}_x/\text{SiN}_x$ as a hard mask. Texturing was performed in TMAH: $\text{H}_2\text{O} = 1: 20$ solution with commercial surfactant at 80°C . The hard mask, after texturing, was then dissolved in HF: $\text{HCl}: \text{H}_2\text{O} = 1: 1: 20$ solution.

C. Fabrication of Silicon Heterojunction Devices With Interdigitated Back Contacts (SHJ-IBC)

The flat rear of the single-side-textured wafers was coated with PECVD (i/p) a-Si:H and PECVD SiO_x hard mask before photolithography, dry etching, and lift-off steps that define the interdigitated pattern. Passivation of the front surface by (i) a-Si:H and SiN_x antireflection coating (ARC) was followed by sputtering indium-doped tin oxide (ITO) and evaporating Cu on the rear to form the electrodes. Lithography and wet etching were again performed to achieve electrical isolation between the contacts. For more details on the rear-side patterning, the reader can refer to our previous publications on the subject [63]–[65].

D. Cell Characterization

Current density (J)–voltage (V) measurements of solar cells were performed under standard testing conditions (AM 1.5G 1000 W/m^2 solar spectrum and 25°C temperature) using a WACOM solar simulator. The WACOM simulator was calibrated before measurements using an externally certified SHJ-IBC cell. Reflectance (R) and external quantum efficiency (EQE) measurements were made using the LOANA solar cell analysis system from PV tools GmbH, with an illumination spot size of $1.5 \times 1.5 \text{ cm}^2$. Samples were prepared for transmission electron microscopy (TEM) measurements as detailed in Appendix B.

III. RESULTS AND DISCUSSION

A. Investigated Pyramid Textures

Scanning electron microscopy (SEM) images of the investigated textures are presented in Fig. 1. The NIL process, briefly described in Section II, was applied to realize periodic INP gratings with an 800 nm pitch, in order to target the near-IR part of the incoming spectrum of light. Our nanopatterned inverse pyramids feature a square base of a size that is defined by the area filling fraction (AFF) and the grating pitch. The AFF is the ratio of the area with INPs to the total area and is a measure of the width of flat regions adjoining the INPs. Reaching an ideal AFF of unity is theoretically possible with square base patterns but given the variation in the NIL process due to substrate roughness, presence of localized defects, and soft-stamp deformations [61], obtaining near-ideal AFF is experimentally very challenging. In our case, we reached AFFs close to 0.85, which is equivalent to a pyramid base width of $\sim 735 \text{ nm}$. More importantly, the nanopyramid dimensions are comparable with

Fig. 1. SEM images of the textures that were integrated into SHJ-IBC devices. (a) Periodic INP gratings of 800 nm pitch were fabricated by NIL. (b) RP texture formed by alkaline etching serves as the reference.

the wavelength of in-coupled photons so that the wave effects become relevant in the wavelength range of interest. On the contrary, the RP texture comprises much larger pyramids of base width size $\sim 2\text{--}5 \mu\text{m}$ and provides path length improvement for in-coupled photons by refracting them at large angles within the absorber.

B. Adapting the Antireflection Coating Layer Thickness

Both investigated pyramid textures were incorporated on the front side of SHJ-IBC devices, as shown schematically in Fig. 2, with the rear side kept flat for ease in the rear-side patterning steps during cell processing. Process details on the fabrication of these devices are briefly described in Section II and covered more extensively in our previous publications [63]–[65]. With the exception of the front-surface texture and ARC layer thickness, both device types were identical in structure and processed together. The thickness of the SiN_x ARC was adapted for each texture to yield low reflection losses in the $500\text{--}1200 \text{ nm}$ wavelength interval, which corresponds to the transmittance spectrum of the perovskite top cell.

We considered spectrum-weighted reflectance (SWR) as the figure of merit in deciding the optimal SiN_x thickness values, which were controlled experimentally by varying deposition times. The optimization, aimed to minimize the SWR in the stated wavelength range for each texture, was carried out by

Fig. 2. Schematic structures of SHJ-IBC devices are shown for both (a) INP and (b) RP textures.

depositing SiN_x on the textured c-Si samples using different deposition times and measuring the reflectance spectra of these samples, followed by computing the SWR. The condition leading to the lowest SWR for each texture was then selected. The SWR takes the incident photon flux into account and is given by

$$\text{SWR} = 1 - \frac{\int_{\lambda_1}^{\lambda_2} (1 - R) \cdot \varphi_{\text{AM}1.5\text{G}} \cdot \partial\lambda}{\int_{\lambda_1}^{\lambda_2} \varphi_{\text{AM}1.5\text{G}} \cdot \partial\lambda} \quad (1)$$

where λ_1 – λ_2 is the chosen wavelength interval, R is the wavelength-dependent reflection coefficient, and $\varphi_{\text{AM}1.5\text{G}}$ is the AM 1.5G photon flux.

In the wavelength interval of 500–1200 nm in which the perovskite top cell was assumed to behave as a sharp bandpass filter, the minima in SWR values of 5.3% for the INP texture and 6.0% for the RP texture was found during optimization and the corresponding SiN_x thicknesses were determined from TEM cross-sectional images, as shown in Fig. 3. The optimal deposition time for the INP texture was found to be shorter, and consequently, the average thickness of SiN_x on the INPs was lower (between 40 and 75 nm) in contrast with that on the RP texture (uniformly ~75 nm). This difference in the optimal thickness could be explained by the choice of grating pitch for the INP texture, meant to target near-IR wavelengths for tandem operation, consequently leading to higher R losses in the intermediate wavelength range (500–800 nm), which is tackled by implementing a slightly thinner ARC layer to target this wavelength range. Moreover, it can be observed from TEM images that unlike the case of the RP texture, SiN_x is nonconformal and

Fig. 3. TEM cross-sectional images showing SiN_x thickness on pyramid facets for (a) INP and (b) RP textures. SiN_x ARC is nonconformal and thinner on the facets of the nanopyramid pattern.

shows thickness variation along the nanopyramid topography, varying uniformly between ~75 nm on the plateaus and ~40 nm in the valleys of the nanopyramids. The nonconformality arises due to the nanopyramid topography, which consists of pyramidal “dents” as opposed to outward projecting pyramids in the case of RPs. This variation in the deposition rate can be explained by the diminished influx of reactant species to the constrained pyramid valleys or conversely because of the slower desorption of reactant products. Therefore, lowering the surface temperature and deposition power may lead to more conformally deposited SiN_x films on nanopyramid-textured surfaces [68] but require a thoughtful optimization as other properties of the film may be affected.

C. Solar Cell Results in Single-Junction and Tandem Operations

J – V parameters of SHJ-IBC solar cells, featuring an ARC optimized to minimize R losses in the 500–1200 nm wavelength interval and an active area of 3.97 cm², are given in Fig. 4 and Table I for S-J operation under the standard AM 1.5G

Fig. 4. Comparison of illuminated J - V results of SHJ-IBC devices with an area of 3.97 cm^2 in S-J operation under the AM 1.5G spectrum with INP and RP surface textures. RP-textured cells reached higher efficiencies.

TABLE I
SUMMARY OF ILLUMINATED J - V RESULTS OF SHJ-IBC DEVICES IN S-J OPERATION FOR BOTH INVESTIGATED SURFACE TEXTURES

Text.		J_{SC} (mA/cm^2)	V_{OC} (mV)	FF (%)	η (%)
INP	Avg. of 7	41.27 ± 0.36	715 ± 7	72.9 ± 0.9	21.5 ± 0.6
RP	Avg. of 11	41.64 ± 0.08	726 ± 2	74.8 ± 0.7	22.6 ± 0.3
INP	Best	41.63	721	74.1	22.3
RP	Best	41.77	729	75.8	23.1

illumination spectrum and testing conditions. As expected for S-J configuration, the INP patterned cells were outperformed by their RP-textured counterparts. Outstanding V_{OC} values above 700 mV have been achieved for both texture types, proving that INP patterning of the surface does not significantly compromise the passivation quality [58]. The slightly lower V_{OC} and fill factor (FF) values for the INP pattern were due to larger nonideal recombination (J_{02}) losses, which we believe could be attributed to RIE-induced surface damage during NIL patterning (step 6 in Appendix A), and the nonconformal intrinsic (i) a-Si:H layer thickness. The latter exhibits a similar nonconformality in thickness as was observed in the case of PECVD SiN_x , which makes it thinner in the valleys than our required target thickness of 5 nm for adequate chemical passivation (see Appendix C). Thus, there is room for further improvement in the V_{OC} and FF of INP-textured cells by improving the conformality of the front side (i) a-Si:H passivation layer. Nevertheless, our best INP patterned device reached an excellent cell efficiency (η) of 22.3% compared with 23.1% for the RP-textured reference in standalone operation under a full AM 1.5G spectrum.

In order to understand the relative optical performance of the two investigated textures in the different regions of the spectrum, we conducted R and EQE measurements on representative devices of both types of texture (see Fig. 5), which revealed that the escape losses for wavelengths between 950 and 1200 nm were much lower in the case of INP texture with an SWR of 13.6% as opposed to 18.7% for the RP texture, translating into a potential J_{SC} gain of $0.50 \text{ mA}/\text{cm}^2$ for this wavelength range. However, the actual J_{SC} gain from EQE results in the stated wavelength interval turns out to be $0.60 \text{ mA}/\text{cm}^2$, which points to additional optical advantage of INP patterning besides superior IR photon trapping. We postulate that the excitation of higher

Fig. 5. (a) Representative SHJ-IBC devices were selected from each texture split for R and EQE comparison in S-J operation. (b) Nanopatterned SHJ-IBC device shows superior IR performance than its RP-textured analog.

order modes by the nanopyramid grating texture may yield lower parasitic absorption losses in the rear-side ITO and Cu contacts from the higher angle light in-coupling it provides. Nonetheless, further investigation is required to identify the reason behind the observed discrepancy of $0.10 \text{ mA}/\text{cm}^2$ between R and EQE measurements.

Although Fig. 5(b) also shows that the RP texture provides better light in-coupling at shorter wavelengths ($<550 \text{ nm}$) compared with an INP grating of 800 nm pitch, these wavelengths are not relevant in the context of a c-Si bottom cell in tandem configuration.

Fig. 6. (a) Schematic structure of a planar perovskite device without contacts that was placed on top of SHJ-IBC bottom cells for EQE and J - V measurements in 4-T tandem operation. The transmitted spectrum reaches the bottom c-Si cell through an airgap. (b) EQE spectra of SHJ-IBC cells underneath a perovskite device precursor of transmittivity (T). The IR boost with nanopatterning was also observed in the 4-T tandem operation.

TABLE II
ILLUMINATED J - V RESULTS OF SHJ-IBC DEVICES IN TANDEM OPERATION

Text.	Config.	J_{sc} (mA/cm ²)	V_{oc} (mV)	FF (%)	η (%)
INP	S-J	41.46	721	73.6	22.1
RP	S-J	41.49	725	74.7	22.5
INP	Tandem	17.86	692	76.8	9.5
RP	Tandem	17.33	693	77.9	9.3

J - V parameters of both devices in S-J operation are also shown for reference.

The efficiency enhancement due to the INP texture in 4-T tandem configuration was then analyzed by measuring the illuminated J - V and EQE characteristics of these SHJ-IBC cells under the filtered AM 1.5G spectrum, placing them beneath a planar perovskite top-cell precursor of n-i-p structure that features all supporting layers except the contacts [see Fig. 6(a)]. In this 4-T configuration, an airgap was present in between the subcells. Since the perovskite absorber layer with an optical bandgap of ~ 1.7 eV is transparent to IR wavelengths, we can assume that the reflected IR light from the bottom cell would partially be parasitically absorbed in the supporting layers of the top cell and the remainder would escape the tandem structure from the front side. Shorter wavelengths below 550 nm, on the other hand, do not reach the bottom cell as they are absorbed by the top cell during the first pass. Consequently, the contribution of light that is redirected to the top cell from the bottom cell was neglected and the scope of the study was limited to the adaptation of bottom-cell design in 4-T tandem configuration. The EQE results in Fig. 6(b) and illuminated J - V results in Table II present that by using an INP texture, the J_{sc} and the η of c-Si bottom cell are higher than when using an RP texture in tandem configuration. It needs to be emphasized that the J_{sc} increment of 0.53 mA/cm² with respect to the RP texture benchmark in tandem operation was obtained using an INP grating with nonideal AFF. Therefore, we suspect that the improvement could be enhanced by accomplishing even higher AFFs or by introducing double-side gratings [62].

IV. CONCLUSION

In this article, we demonstrated increased IR absorption in SHJ-IBC by integrating INP gratings. The gratings were prepared by NIL and compared with state-of-the-art RPs as the front-side texture to trap IR photons, with a view to their application in c-Si bottom cells in a 4-T perovskite/c-Si tandem device. Our cell results show that by using a grating pitch of 800 nm and tweaking the ARC layer thickness, improvement in IR absorption is offset by inferior light in-coupling at

shorter wavelengths and leads to an overall reduced performance compared with the RP texture in S-J operation under the AM 1.5G spectrum. However, the IR absorption enhancement with nanopatterning becomes relevant when considering bottom-cell design for 4-T tandem devices. In our case, replacing the RP texture by INP gratings provided a short-circuit current density gain of 0.53 mA/cm² and elevated the bottom-cell efficiency.

APPENDIX A
SCHEMATIC PROCESS FLOW OF THE THERMAL NIL PROCESS
TO FABRICATE INP GRATINGS

APPENDIX B
TEM SAMPLE PREPARATION

TEM sample preparation consists of the following steps.

- 1) Spin-on Carbon (SoC) is deposited on the die before the sample enters the focused ion beam (FIB). At the FIB, Pt is deposited on the region of interest (and on top of SoC) by ion beam deposition. The FIB uses Ga ions to mill around the region of interest (now covered by SoC + Pt) so that a cross section is extracted from the sample.
- 2) The extracted cross section is lifted away from the die and attached to a Cu grid.
- 3) The extracted cross section is thick ($\sim 3 \mu\text{m}$) and is further thinned using also the Ga ion beam until the cross section is < 100 nm thick. In this step, both the back and front sides of the cross section are thinned an equal number of times until a thickness of < 100 nm is achieved. This is carried out using Ga ions at 5 kV. The cross section is thinned by moving the Ga ion beam downward from the top to the bottom of the sample.

APPENDIX C LOSS IN CHEMICAL PASSIVATION IN THE VALLEYS OF NANOPYRAMIDS

(i) a-Si:H layer thickness at the nanopyramid plateaus

(i) a-Si:H layer has non-optimal thickness within the nanopyramid valleys

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