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Assessment of Bulk and Interface Quality for Liquid Phase Crystallized Silicon on Glass

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Abstract—This work reports on the electrical quality of liquid phase crystallized silicon (LPC-Si) on glass for thin-film solar cell applications. Spatially resolved methods such as light beam induced current (LBIC), microwave photoconductance decay (MWPCD) mapping and electron backscatter diffraction (EBSD) were used to access the overall material quality, intra-grain quality, surface passivation and grain boundary (GB) properties. LBIC line scans across GBs were fitted with a model to characterize the recombination behavior of GBs. According to MWPCD measurement, intra-grain bulk carrier lifetimes were estimated to be larger than 4.5 μs for n-type LPC-Si with a doping concentration in the order of 10^{16} cm^{-3} . Low-angle GBs were found to be strongly recombination active and identified as highly defect-rich regions which spatially extend over a range of 40–60 μm and show a diffusion length of 0.4 μm . Based on absorber quality characterization, the influence of intra-grain quality, heterojunction interface and GBs/dislocations on the cell performance were separately clarified based on 2D-device simulation and a diode model. High back surface recombination velocities of several 10^5 cm/s are needed to get the best match between simulated and measured open circuit voltage (V_{oc}), indicating back surface passivation problem. The results showed that V_{oc} losses are not only due to poor back surface passivation but also due to crystal defects such as GBs and dislocation.

Index Terms—Liquid phase crystallized silicon, light beam induced current, bulk lifetime, heterojunction, grain boundaries, 2D-device simulation.

I. INTRODUCTION

ONE of the strategies to further reduce solar cell costs is to employ very thin absorber materials with high

electronic quality, such as thin monocrystalline or multicrystalline silicon ideally directly processed on glass substrates. Thin multicrystalline silicon films on glass formed by melt induced crystallization of silicon precursors using a line shaped energy source, known as liquid phase crystallized (LPC) silicon [1], [2], have been proven as a promising material for solar cells as shown by the remarkable high open circuit voltages of up to 661 mV [3]–[5]. This crystallization technique offers a low energy demand respect to area almost 3 times lower than that for wafer based approaches [3]. Interdigitated back-contact silicon heterojunction (IBC-SHJ) solar cells based on conventional silicon wafers reached an efficiency of 26.7% [6] showing the potential of this contact system to approach the theoretical efficiency limit of 29% [7]. IBC-SHJ structures have been successfully applied to LPC-Si on glass and an efficiency of 14.2% was achieved for 13 μm -thick- absorber [4]. For back contact systems, the balance between electrical shading and resistive losses is one of the key factors to maximize the electrical performance of the cells. It has previously been shown that n-type LPC-Si based cells with a doping concentration (N_d) of $3 \times 10^{16} \text{ cm}^{-3}$ and an electron collector finger width of 120 μm and hole collector finger width of 1080 μm are optimum for achieving the highest average cell efficiency [5], [8]. The record cell exhibits an efficiency of 14.2% with this contact geometry and doping concentration (N_d) of $8 \times 10^{16} \text{ cm}^{-3}$ [4]. A current loss analysis based on light beam induced current (LBIC) and electroluminescence (EL) is presented in [8] and [9] and reports a loss in short circuit current density of up to 4.0 mA/cm^2 and 2.9 mA/cm^2 due to crystal defects and the electron collector region, respectively. Therefore, additional methods to access the material quality, the LPC-Si/heterojunction interface and grain boundary properties are needed to further explore the potential of the IBC-SHJ cell based on this material.

Different attempts to approach the silicon quality were applied such as quasi-steady state photoconductance (QSSPC), transient photoconductance decay (PCD), transient photoluminescence (TR-PL), photoluminescence imaging and evaluation of the internal quantum efficiency (IQE) using 1D and 2D simulations [10], [11]. However, special care has to be taken when applying common wafer-based characterization

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techniques to LPC-Si. For examples, for the QSSPC method the signal to noise ratio is very low due to the limited thickness of the film and for PL special care has to be taken to avoid detrimental effects caused by glass luminescence [10]. Thus, the evaluation of the IQE using device simulators has proven to be a suitable method [10]. A first comprehensive investigation of the absorber quality was presented in [11] applying high resolution LBIC for investigating the lateral quality and using 2D-simulation to estimate the material quality. For simplification, recombination at the SHJ was omitted in the study due to the excellent passivation properties of this structure. In this work, we combine microwave photoconductive decay (MWPCD) mapping, LBIC and 2D simulations to assess all recombination pathways of LPC silicon. MWPCD provides images of the effective minority carrier lifetime of LPC-Si passivated with an a-Si:H (i/p+) layer stack, while an LBIC scan reveals the spatial distribution of carrier collection across the fully contacted cells. For the investigation of grain boundaries (GBs), electron back scatter diffraction (EBSD) was used to determine the GB types. Additionally, GBs were also characterized by recombination velocities and defect regions based on fitting LBIC line scan of GBs with models developed by Micard *et al.* [12].

Unlike solid phase crystalline silicon or metal induced crystallized silicon, which have grain sizes in micrometer range [13], [14], LPC-Si material has grain size is up to centimeters in length and a few millimeters in width. According to LBIC records [8], the intra-grain quality is almost homogeneous, independent on grain orientation, and the fraction of intra-grain area to the total cell area contributes significantly to current gain (Fig. 2 top). Therefore, it is necessary to investigate the effect of intra-grain and GBs/dislocations on cell performance separately to clarify loss mechanisms. To meet this purpose, we first discuss on J_{sc} and V_{oc} loss in intra-grain regions by modeling a 2D-device using TCAD-SentaurusTM simulation tool [15]. For this simulation, absorber quality was assumed to be equal to intra-grain quality and back surface recombination velocities were varied until simulated V_{oc} match measured V_{oc} . Additionally, 2D-device simulation was also performed for the cell with absorber quality like the quality of GBs/dislocations as characterized by fitting LBIC line scan profile models. Finally, the LPC-Si cell performance was estimated by combining two devices (intra-grain-like quality device and GBs/dislocations-like quality device) as two diodes connecting in parallel with appropriate area factors estimated from LBIC.

II. EXPERIMENTAL PROCEDURE

A. Absorber and cell fabrication

15 μm -thick n-type LPC-Si films were formed on glass substrates by liquid phase crystallization using a line-shape continuous wave diode laser (808 nm) at a scan speed of 3 mm/s. Plasma-enhanced chemical vapor deposition (PECVD) of $\text{SiO}_x/\text{SiN}_x/\text{SiO}_x\text{N}_y$ stacks, in which the SiO_xN_y was formed by plasma oxidation of the SiN_x film, were used as multi-functional intermediate layers (ILs) between glass and LPC-Si [16]. Besides serving as an adhesion and impurity

diffusion barrier during crystallization, they provide an excellent surface passivation and an anti-reflective coating property at the front. Absorber doping was achieved by subsequent PECVD deposition of an a-Si (n) layer using an adjusted phosphine flow rate. Cells with doping concentration (N_d) range of 10^{16} cm^{-3} were investigated in this work since this doping range gives a good balance between J_{sc} and V_{oc} [1], [17]. Samples were then capped with a PECVD SiO_x layer and subsequently crystallized under vacuum conditions. Details on the sample preparation and crystallization process are described in ref [1]. In order to passivate crystallographic defects in the liquid phase crystallized absorbers, the samples were exposed to a hydrogen plasma treatment with a H_2 flow of 50 sccm and a power of 50 W at 600 °C for 15 min. Details of this process can be found in [18], [19]. After the hydrogenation process, the back surface of LPC-Si films was textured with a potassium hydroxide (KOH)-based solution. IBC-SHJ cells were fabricated on $5 \times 5 \text{ cm}^2$ substrates using three photolithography steps, following processes described in ref [4]. The hole collector (a-Si:H(p+)) as well as the electron collector (a-Si:H(n+)) were deposited using the PECVD method. For interface passivation between LPC-Si and the hole collector an intrinsic amorphous silicon (a-Si:H(i)) layer was added. An aqueous solution consisting of hydrofluoric acid (HF), nitric acid (HNO_3), and phosphoric acid (H_3PO_4) was used to etch the a-Si:H(i/p+) layers. The a-Si:H(n+) film was etched using the selective etchant tetramethylammonium (TMAH). We used 20% hydrochloric acid (HCl) for ITO etching and a diluted mixture of ammonia solution (NH_4OH) and hydrogen peroxide (H_2O_2) for silver (Ag) etching. The cross section of an IBC-SHJ cell is shown in Fig. 1. Finally, the IBC LPC-Si solar cells were annealed at 180 °C for 20 minutes.

Fig. 1. Cross-sectional scheme of an IBC-SHJ cell based on LPC-Si on glass.

We prepared several batches of samples to investigate the impact of N_d and contact geometry on the cell performance. The full dataset of $J(V)$ parameters can be found in [5] and [8]. In this study, for the subsequent material quality assessment, we concentrate on the three best-performance cells with N_d of $3 \times 10^{16} \text{ cm}^{-3}$ (cell A), $8 \times 10^{16} \text{ cm}^{-3}$ (cell B) and $12 \times 10^{16} \text{ cm}^{-3}$ (cell C) with a width of the hole and electron collector fingers of 1080 and 120 μm , respectively.

For carrier lifetime measurements, $2 \times 2 \text{ cm}^2$ LPC-Si on glass samples with N_d of 3×10^{16} and $12 \times 10^{16} \text{ cm}^{-3}$ were prepared. The back surface of samples was covered with a-Si:H (i/p+) layers which are same as passivation and hole collector layers used for IBC-SHJ cell fabrication.

B. Cell characterization

The doping concentration of the samples was calculated via the sheet resistance, which was determined by a four point probe measurement (Jandel RM3-AR). Hole and electron mobilities were assumed to be 80% of the hole and electron mobilities in FZ-Si. Current-voltage (J - V) curves were obtained using an AAA rated solar simulator of type Wacom WXS-156S-L2, AM1.5GMM with dual light sources (halogen and xenon lamp). Reflection (R) and transmission (T) spectra were measured with a PerkinElmer LAMBDA 1050 spectrophotometer.

LBIC measurements were conducted using a self-built set-up at the University of Ljubljana [20]. The measurement was conducted with a 638 nm-wavelength laser light. For an overview scan of the total cell area, the spot size was $60 \mu\text{m}$ in diameter and the step was $30 \mu\text{m}$ (except for sample A, the step was $50 \mu\text{m}$, spot size was $120 \mu\text{m}$). For small area, step of $5 \mu\text{m}$ and spot size of $25 \mu\text{m}$ was used. PL measurements were set up with an array of 650 nm-wavelength diode lasers to illuminate the sample at 1 sun intensity. The image was recorded with a silicon CCD camera. Minority carrier lifetimes were mapped by the microwave photo-conductance decay (MWPCD) method with a 349 nm laser which generated a photon density of $4 \times 10^{12} \text{ cm}^{-2}$. The excess carrier concentration of $7.8 \times 10^{16} \text{ cm}^{-3}$ is estimated for measured samples. The laser spot size was 2 mm . The signal was measured with step sizes of 0.5 mm and a microwave frequency of 26 GHz . For GB investigations, electron backscatter diffraction (EBSD) was used. EBSD maps were acquired at a step size of $15 \mu\text{m}$ using an Oxford Instruments NordlysNano camera attached to a Zeiss UltraPlus scanning electron microscope. The acceleration voltage and the beam current were 15 kV and about 1 nA , respectively.

C. Device simulation

2D-device simulations were performed using TCAD-SentaurusTM simulation tool from Synopsys[®] [15]. The input electrical parameters for a-Si layers are standard values taken from literature and measurement values compiled in AFORS-HET [21]. For LPC-Si, we modified the literature values compiled in AFORS-HET according to measurement result to match lifetime, mobility and doping density. All input parameters used in this work are summarized in Table A-I in Appendix. Photon generation profile was calculated using equation developed in literature [4] and the absorption in $13 \mu\text{m}$ -thick c-Si absorber extracted from Genpro4 simulation [22]. Optical data of interlayer stacks and ITO used for Genpro4 simulation were determined by spectroscopic ellipsometry measurement. The generation profile was confirmed by 2D-device simulation using idealized structures and comparison of the simulated photocurrent with the value achieved by Genpro4.

III. RESULTS

A. Light beam induced current measurement

For material quality assessment, LBIC images were recorded for the IBC-SHJ cells with N_d of 3×10^{16} (cell A), 8×10^{16} (cell B) and 12×10^{16} (cell C). One can see in Fig. 2 that the current loss is mainly attributed to electrical shading at the electron collector and to high carrier recombination at crystal defects such as grain boundaries and stacking faults. There are GBs with a lateral extension of over $100 \mu\text{m}$ in width which show high carrier recombination. According to our EBSD analysis, these are low-angle GBs. High-angle GBs are less detrimental and exhibit a width of less than $50 \mu\text{m}$. Details on GB characterization are discussed in section III.D.

Fig. 2. LBIC (top) and PL (bottom) of cells A, B and C. In LBIC images, gray images are some crystal defects scanned with a step size of $5 \mu\text{m}$ for better resolution. LBIC signals of some GBs/dislocations in cell A are discontinuous because the cell was measured with laser spot radius smaller than step.

By counting the pixel areas according to the LBIC signal value/intensity, current losses from electron collector fingers and GBs/dislocations were evaluated. The cell area, electron collector fingers and GBs/dislocations areas were estimated based on the following approaches:

(1) Carrier collection area (bright area) was estimated by setting a threshold value (for example, threshold signal for cell B is signal larger than 85%). This method will cause overestimation of area because a threshold higher than 50% was chosen to include the relevant features. Therefore we estimated this error on the borders of the cell and electron collector finger, and corrected the carrier collection area accordingly, due to influence of counting border pixels. In order to avoid this effect, estimation error was calculated by correction area calculated with border threshold of 50%.

(2) The electron collector width and height were extracted from vertical and horizontal averaged line scans through the respective locations. For this calculation, the amount of pixels was evaluated based on the drop of signal intensity with 50% threshold.

(3) Cell area was calculated using width and height of the cells extracted from profiles of vertical and horizontal line scan through the cell, also with 50% threshold.

The sum of measured J_{sc} and anticipated dark area total current loss is approximately 33 mA/cm^2 for all cells. This value matches the potential J_{sc} obtained from optical simulations using Genpro4 [22] for $13 \mu\text{m}$ thick LPC-Si films which include losses from reflectance and parasitic absorption

Table I
SUMMARY OF J_{sc} , L_{eff} , τ_{eff} AND SRV OF THE CELLS
INVESTIGATED IN THIS WORK

Parameter/cell	A	B	C
N_d [cm^{-3}]	3×10^{16}	8×10^{16}	12×10^{16}
Measured J_{sc} [mA/cm^2]	26.9	26.5	27.1
Total dark area [%]	18.6	20.2	17.2
Dark area at electron collector fingers [%]	7.9	8.2	8.8
Estimated J_{sc} without losses [mA/cm^2]	33	33.1	32.8
Total J_{sc} loss [mA/cm^2]	6.1	6.5	5.9
Estimated J_{sc} loss at electron collector fingers [mA/cm^2]	2.6	2.7	2.9
Estimated J_{sc} loss by crystal defects [mA/cm^2]	3.5	4.0	2.8
Estimated J_{sc} without losses from crystal defects or Estimated J_{sc} of intra-grain cell [mA/cm^2]	30.4	30.5	29.8
L_{eff} of intra-grain above electron collector region [μm]	19.1 ± 2.7	14.7 ± 1.3	13.2 ± 0.8
Maximum τ_{eff} of intra-grain above hole collector region [μs]	7.8	x	3.6
Minimum τ_{bulk} of intra-grain [μs]	13.4	x	4.5
L_{eff} of intra-grain above hole collector region [μm]	79	x	48
SRV_{front} [cm/s]	70	70	70
Simulated V_{oc} [mV] with $SRV_{back} < 10^3$ [cm/s]	690	710	705
Simulated J_{sc} [mA/cm^2] with $SRV_{back} < 10^3$ [cm/s]	32.1	31.7	30.8
Measured V_{oc} [mV]	636	650	646
Measured V_{oc} for test cell [mV]	x	670	x
Estimated V_{oc} of intra-grain cell [mV]	650	670	665
SRV_{back} at intra-grain/hole collector interface used to fit V_{oc} and J_{sc} of intra-grain cell (cm/s)	3×10^5	1.5×10^5	1.5×10^5
SRV_{back} at intra-grain/electron collector interface V_{oc} and J_{sc} of intra-grain cell (cm/s)	6×10^6	1.2×10^6	1.2×10^6
Simulated J_{sc} of GBs/dislocation cell [mA/cm^2]	0.52	0.59	0.50
Simulated V_{oc} of GBs/dislocation cell [mV]	355	320	360
Simulated J_{sc} using diode model [mA/cm^2]	27.2	26.9	27.2
Simulated V_{oc} using diode model [mV]	634	652	652

in ITO and glass [5]. This indicates that almost all carriers generated in non-defective grain areas in the hole collector

region were collected. Current loss due to crystal defects is in range of 2.8-4.0 mA/cm^2 , depending on the amount of GBs/ dislocations in the cell. GBs/ dislocations result in a current loss of $\geq 2.8 \text{ mA}/\text{cm}^2$, which was also observed in previous reports on LPC-Si [9], [11], [23] with intermediate layers as $\text{SiO}_x/\text{SiN}_x/\text{SiO}_x$ or $\text{SiN}_x/\text{SiO}_x/\text{SiO}_x\text{N}_y$ stacks. The number of these GBs/ dislocations, especially strong carrier recombination active defects such as stacking faults, twin boundaries and low-angle GBs, can be reduced by optimized precursor deposition or crystallization processes [5]. At electron collector fingers, current loss are 2.6, 2.7 and 2.9 mA/cm^2 for cell A, B and C, respectively. By adding measured J_{sc} with current loss to GBs/ dislocations, J_{sc} without losses from GBs/ dislocations of 30.4, 30.5 and 29.8 mA/cm^2 were estimated for cell A, B and C, respectively, as listed in table I. The estimated J_{sc} of cell A is lower than that of cell B. It is might be due to J_{sc} overestimation due discontinuous GBs signal from LBIC image because cell A was measured with laser spot radius smaller than step. These J_{sc} values are considered as estimated J_{sc} of LPC-Si intra-grain cells for further discussions in this work.

By fitting LBIC line scans across all electron collector fingers with the collection probability function [9], [11] the effective minority carrier diffusion lengths (L_{eff}) of LPC-Si above the electron collector were estimated to be $(19.1 \pm 2.7) \mu\text{m}$, $(14.7 \pm 1.3) \mu\text{m}$ and $(13.2 \pm 0.8) \mu\text{m}$ for cells A, B and C, respectively. These values are in agreement with published diffusion lengths in LPC-Si material due to the same a-Si:H (n^+) layers [9]. L_{eff} is limited by the bulk quality of LPC-Si material and an poor surface passivation at the LPC-Si/ electron collector interface caused by the absence of an a-Si:H (i) passivation layer. As one can see in PL images (Fig. 2 bottom), the hole collector area looks brighter compared to electron collector area, indicating reasonable passivation at the hole collector/LPC-Si interface thanks to a-Si:H (i) layer. At LPC-Si region above electron collector, L_{eff} is smaller than a half of the electron collector finger width for all doping concentrations. Therefore, carrier collection is poor here, causing a current loss of 2.6-2.9 mA/cm^2 as mentioned above.

B. Effective carrier lifetime mapping of LPC-Si passivated by a-Si:H (i/p+) layer

To evaluate passivation quality of a-Si:H (i/p+) layer on LPC-Si absorbers, effective carrier lifetimes (τ_{eff}) of LPC-Si samples passivated only by a-Si:H (i/p+) layer were measured by MWPCD. τ_{eff} mappings and corresponding histograms are shown in Fig. 3. Please note that these lifetime mappings were measured with a laser spot of 2 mm and a step size of 0.5 mm. Thus, the spatial resolution is much lower compared to the LBIC maps. Therefore, GBs and dislocations can't be visualized. However, one can distinguish regions with lower and higher τ_{eff} . We assume that the lower τ_{eff} region includes signal of GBs/dislocation, and the higher τ_{eff} region corresponds to a signal from an intra-grain region where no GBs are included. LBIC records indicate that all grains have the same quality. For that reason the highest measured τ_{eff} were assigned to the intra-grain regions, i.e. 7.8 μs and 3.6 μs are assumed to be the highest τ_{eff} of LPC-Si intra-grains passivated by a-Si:H (i/p+) layer of cell A ($N_d = 3 \times 10^{16} \text{ cm}^{-3}$)

and cell C ($N_d = 12 \times 10^{16} \text{ cm}^{-3}$), respectively. This corresponds to an effective diffusion length within the emitter region of 79 μm and 48 μm for cells A and C, respectively, calculated using the equation (1). This value is almost 2-4 times higher than L_{eff} at absorber region above electron collector determined by fitting LBIC line scan profile and highlights the important role of the a-Si:H (i) layer for back surface passivation.

Fig. 3. τ_{eff} mapping of LPC-Si/a-Si:H(i/p+) samples with N_d corresponding to cell A (left) and C (right) with corresponding histograms. Samples were measured in superstrate configuration for $1 \times 1 \text{ cm}^2$ area

C. Intra-grain cell performance

Fig. 4. $J(V)$ curve of small test cell. The inset shows the PL image of the cell.

To rule out the effect of GBs/ dislocations on the open circuit voltage, a small test cell with the size of $1.5 \times 1.5 \text{ mm}^2$ was fabricated on a single crystalline area. This cell was fabricated in parallel with the IBC-SHJ cells. This test cell exhibits the same doping concentration as cell B ($N_d = 8 \times 10^{16} \text{ cm}^{-3}$), but the cell area is comprised of only the hole collector. Hole collector area was designed as $1.5 \times 1.5 \text{ mm}^2$ on lithography mask. Because of over etching during photolithography processes, the area was $1.47 \times 1.47 \text{ mm}^2$, measured by microscope measurement. However, it is

challenging to determine the exact active area of small cell. Therefore, V_{oc} reliably demonstrates the cell performance but J_{sc} reliability is subject to the area estimation error. As shown in Fig. 4, a V_{oc} of 670 mV was achieved, which is 20 mV higher than cell B. LBIC images in Fig. 2(top) indicates homogeneous intra-grain quality. This suggests that GBs/dislocations cause a reduction of 20 mV in V_{oc} . Measured J_{sc} of this cell is 32.3 mA/cm^2 , which is much higher than measured J_{sc} of cell B, since here is no current loss from GBs/dislocation and from electrical shading. For cell B, J_{sc} without this losses is 33 mA/cm^2 estimated from LBIC (Table I). The difference of 0.7 mA/cm^2 probably arises from estimation error for active area of the small test cell as mentioned above.

D. Grain boundary characterization

In order to understand GBs in terms of boundary type and grain orientation, we used EBSD (Fig. 5 right) to investigate the GB types of a LPC-Si sample. We found that regions with high recombination (dark) in the PL image (Fig. 5 left) are assigned to low-angle GBs (misorientation angle of less than 15°) and stacking faults. It is reported that low-angle GBs are effective gettering sites for impurities due to their particular boundary dislocation structure, thus, they are strongly recombination active [24], [25]. Twin boundaries do not affect the PL signal substantially.

Fig. 5. PL image (left) and EBSD image with color coding of different crystallographic directions (right) of a LPC-Si sample.

In order to quantify the recombination at GBs, we used a model established by Micard *et al.* [12] to determine the recombination velocity (RV) at GBs in LPC-Si by fitting LBIC line scan signals across GBs with a simulated profile. In the model, recombination at GBs is described as an interface recombination velocity or a defect layer between two neighboring grains. The induced current is calculated based on the excess carrier density solved from the diffusion equation at steady state conditions. The current profile was normalized to a plateau value at a point in the grain far away from GBs. More details about this model and the theory are described in refs [12] and [26]. For the minority diffusion lengths of neighboring grains, the previously determined values of L_{eff} for intra-grain passivated by a-Si:H (i/p+) layers were assumed.

For high-angle GBs, RV 's in the range of 10^4 - 10^5 cm/s were found. Using the same method, RV 's in the range of 10^3 to 5×10^4 cm/s were quantified for the majority (90%) of GBs in Si-wafers, [27]. Lower RV 's on the order of 10^3 cm/s were reported for GBs by fitting PL signals [28], [29]. However, the accuracy of this method depends strongly on the resolution of the PL image and optical properties of samples. By evaluating EBIC line scans, RV 's of $\sim 10^5$ cm/s were obtained for GBs [30], which is in good agreement with the results of this study. For low-angle GBs, a defect region model needs to be used to get good fitting. A reasonable fit was achieved using a defect-rich region with a width of 40-60 μm and diffusion length of 0.4 μm . Examples for fitted LBIC profiles of GBs in LPC-Si are shown in Fig. 6. It was found that the properties of GBs do not depend on the doping concentration but on the type of the GB.

Fig. 6. Fitting LBIC signals of two high-angle GBs in LPC-Si using recombination velocities of 3×10^4 and 2×10^5 cm/s and a low-angle GB using defect region with a width of 47 μm and diffusion length of 400 nm. Fitting models were developed by Micard *et al.* [12].

E. Simulation results

E.1. LPC-Si intra-grain quality and back surface passivation

2D-device simulations were performed to access to loss mechanisms of LPC-Si intra-grain regions. Effective carrier lifetimes measured by MWPCD are combination of bulk quality and surface recombination. As mentioned in section III. B, these measured lifetimes could be also affected from GBs/dislocation. Therefore, taking average value of measured lifetime is not a proper way to evaluate intra-grain bulk quality. Due to this reason, the highest τ_{eff} values in mapping lifetime were taken as the highest τ_{eff} of intra-grains passivated by a-Si:H (i/p+) layer. Assuming that back surface passivation is perfect ($SRV_{\text{back}}=0$ cm/s), minimum bulk carrier lifetimes (τ_{bulk}) of 13.4 and 4.5 μs are obtained for the intra-grain quality of cell A and cell C, respectively, following the equation:

$$\frac{1}{\tau_{\text{eff}}} = \frac{1}{\tau_{\text{bulk}}} + \frac{SRV_{\text{front}} + SRV_{\text{back}}}{H} \quad (2)$$

where H is the thickness of the absorber and τ_{eff} of 7.8 μs and 3.6 μs were used for cell A and cell C, respectively.

Using these τ_{bulk} values, τ_{bulk} of 10 μs was interpolated for intra-grain in cell B using a doping dependent Shockley-Read-Hall (SRH) lifetime, based on the Scharffeter model [31].

Fig. 7. Simulated J_{sc} , V_{oc} and FF as a function of SRV_{back} at the LPC-Si intra-grain/hole collector and LPC-Si intra-grain /electron collector interfaces.

Front surface recombination velocity (SRV_{front}) at the interface between LPC-Si intra-grain and the ILs was evaluated in literatures [4], [16], [23], [32]. Preissler *et al.* investigated SRV_{front} using the extended Shockley Read Hall recombination model and the fixed charge density and interface defect state density determined from capacitance-voltage measurements on developed metal-insulator-semiconductor (MIS) structures [13], [28]. SRV_{front} in the range of 10 to 53 cm/s were estimated for LPC-Si passivated with $\text{SiO}_x/\text{SiN}_x/\text{SiO}_x$ assuming constant capture cross sections taken from literature. On the other hand, SRV_{front} were estimated between 100 to 200 cm/s for LPC-Si passivated with SiN_x and SiO_x from measured cell parameters or LBIC line scans which were modeled using 2D-device simulation or fitting LBIC signal line scans with ASPIN3 [23], [33] and TCAD-SentaurusTM [4], [15]. For this study, an average SRV_{front} of 70 cm/s was used for further investigation.

Up to now, back surface passivation at the hole and electron collector contact is still a hidden factor for LPC-Si material. To get the best matching between measured and

simulated V_{oc} , a defect layer must be implemented into simulation [1], [4], [32]. In this study, we quantified the back surface passivation quality using surface recombination velocity (SRV_{back}). For simplification, we first assumed that SRV_{back} of LPC-Si intra-grain/ passivation layer interface at hole collector region (so called LPC-Si intra-grain/ hole collector interface) is the same as $SSRV_{back}$ of LPC-Si intra-grain/electron collector interface. Simulated J_{sc} and V_{oc} as a function of SRV_{back} are plotted in Fig. 7.

When $SRV_{back} \leq 10^3$ cm/s, simulated V_{oc} values are 690, 710 and 705 mV for cell A, B and C, respectively. Simulated V_{oc} reach measured value of the cells when SRV_{back} is in range of 10^5 - 10^6 cm/s. In this high SRV_{back} range, V_{oc} values are the same for three cells, as shown in Fig 7(b), indicating that V_{oc} is mainly limited by back interface passivation. According to the section III.C, the cell with intra-grain quality exhibited V_{oc} of 670 mV with the same N_d level as of cell B. The same value is obtained for simulated V_{oc} when SRV_{back} is 1.6×10^5 cm/s. The results indicate that approximately 40 mV was lost due to poor back surface passivation.

For cell B, at SRV_{back} of 1.6×10^5 cm/s, simulated J_{sc} is 31.4 mA/cm² which is higher than J_{sc} of intra-grain cell (estimated from LBIC results, 30.5 mA/cm²). Simulated J_{sc} matches this value when SRV_{back} at LPC-Si intra-grain/electron collector exceeds 10^6 cm/s. This is reasonable since there is no a-Si:H(i) layer between LPC-Si intra-grain and the electron collector. The surface passivation quality there should be worse than at LPC-Si/hole collector interface which has the a-Si:H(i) layer in between. By varying values of SRV_{back} of LPC-Si/ hole collector and LPC-Si intra-grain/electron collector interfaces, we can achieve simulated J_{sc} and V_{oc} equal to estimated J_{sc} and V_{oc} for intra-grain cell at SRV_{back} of 1.6×10^5 cm/s at hole collector contact and 1.2×10^6 cm/s at electron collector contact. Simulated J_{sc} with $SRV_{back} \leq 10^3$ cm/s is 31.7 mA/cm² for cell B, as shown in Fig. 7(a) that is 1.2 mA/cm² higher than J_{sc} of intra-grain cell estimated from LBIC result, indicating J_{sc} loss of 1.2 mA/cm² due to poor passivation at LPC-Si/electron collector interface. High SRV_{back} does not cause a significant decrease in FF , as shown in Fig. 7 (c). High simulated FF was obtained since no contact resistance was implemented into simulation. Simulated FF is close to the highest pseudo FF (82%) obtained for real IBC-SHJ cells.

We assume now that 40 mV is also the V_{oc} loss for cells A and C due to poor back surface passivation problem. SRV_{back} at LPC-Si/hole collector and at LPC-Si intra-grain/electron collector interfaces were varied to obtain simulated V_{oc} and J_{sc} as expected for intra-grain quality for cells A and C, i.e. V_{oc} of 650 mV and J_{sc} of 30.4 mA/cm² for cell A and V_{oc} of 670 mV and J_{sc} of 29.8 mA/cm² for cell C. SRV_{back} values at LPC-Si intra-grain/ electron collector and at LPC-Si intra-grain/ hole collector that satisfied the condition are listed in Table I.

E.2. Cell with absorber like grain boundaries/dislocations quality

For GBs cells, we modeled a cell assuming an absorber quality equal to the quality of low-angle GBs, i.e. a diffusion length of 0.4 μ m as characterized by fitting LBIC line scan profile with defect-rich region model in section III.D. Carrier mobilities of 44 cm/Vs [34], which amounts to the field effect

mobility of nanocrystalline silicon were taken into account and a corresponding bulk lifetime of 1.5 ns is calculated based on eq. (1). The simulated J_{sc} and V_{oc} values are listed in Table I. For example, simulated J_{sc} and V_{oc} of 0.52 mA/cm² and 354 mV for cell B as a model for GB/dislocation areas.

IV. DISCUSSION

Based on simulation data and measured V_{oc} of the intra-grain test (full hole collector) cell, we observed a V_{oc} loss and J_{sc} loss, for example, 40 mV and 1.2 mA/cm² for cell B, due to poor back surface passivation. Thus, enhancement in the back surface passivation should be focused in order to achieve the higher cell efficiency. According to LBIC analysis, 2.6-2.9 mA/cm² current loss is due to electrical shading loss. Therefore, at current state of absorber quality as estimated in this work, improvement in LPC-Si/ electron collector interface passivation may be combined with a new geometry of the fingers to prevent completely electrical shading loss.

By comparison of the performance of test cell and IBC-SHJ cell, the influence of GBs/dislocations on J_{sc} and V_{oc} are clearly observed. To analyse the impact of GBs/dislocations in detail, we superimposed crystalline areas and GBs/dislocations as two diodes in parallel connection (multi-diode) by combining the $J(V)$ curves of the two modelled devices with appropriate area factor (A):

$$J(V) = A_{intra-grain} \times J_{intra-grain}(V) + A_{GBs} \times J_{GBs}(V) \quad (3)$$

Area factors for intra-grain and GBs/dislocations of the cells were determined based on LBIC analysis, as shown in Table I. This approach has been used to estimate the cell performance of multi c-Si wafer with bulk carrier lifetime range (1-600 μ s) [35]. Using this approach, the effect of GBs/dislocation can be investigated. $J(V)$ data of intra-grain cell were taken as simulated curves that simulated V_{oc} , and J_{sc} match estimated values for intra-grain cells, as listed in Table I, e.g. 670 mV and 30.5 mA/cm² for cell B. Simulated $J(V)$ data of GBs/dislocation cells were obtained as described in section III.E.2. Superimposing these two cells according to eq. (3) results in a simulated J_{sc} and V_{oc} for LPC-Si cells. These values are listed in Table I as simulated J_{sc} and V_{oc} using diode model. These values match quite well to the experimental J_{sc} and V_{oc} of the real cells, confirming the deteriorating effect of GBs/dislocations on cell performance and the relevant estimation of quality of intra-grain and GBs/dislocation in this work.

In conclusion, approximately V_{oc} loss up to 20 mV and J_{sc} loss up to 4 mA/cm² is due to GBs/dislocation. Thus, decreasing the number of low-angle GBs or preventing activated recombination at GBs is a promising way to further enhance the cell performance.

V. CONCLUSION

We investigated bulk carrier lifetime, back surface passivation and grain boundary properties of LPC-Si on glass based on LBIC, MWPCD, and EBSD characterization accompanied by analytical and 2D numerical simulations.

Bulk carrier lifetime of LPC-Si intra-grain are found to be higher than 4.5 μs for a doping level of 10^{16} cm^{-3} . For samples passivated with a-Si:H(i/p+) layers, minority carrier diffusion length of 48-79 μm were estimated for intra-grain quality. Besides GBs/dislocation, the LBIC signal indicated a poor carrier collection at the electron collector. According to simulation results, a J_{sc} loss of 1.2 mA/cm^2 and V_{oc} loss of 40 mV were observed for LPC-Si cell due to poor back surface passivation. Therefore, enhancement in back surface passivation is necessary to gain higher J_{sc} and V_{oc} . In addition to the loss caused by high recombination at heterojunction interface, GBs/dislocation causes an approximate V_{oc} loss up to 20 mV and J_{sc} loss up to 4 mA/cm^2 . An EBSD image indicates that low-angle GBs are strongly recombinationaly active. By fitting LBIC line scan profiles across GBs, we found that high-angle GBs were quantified by a recombination velocity of 10^4 - 10^5 cm/s while low-angle GBs were characterized by a defect region width of 40-60 μm with a diffusion length of 0.4 μm . Therefore, in addition to improvement in back interface passivation, efforts should be focused on increase in LPC-Si absorber quality, such as, enhancement in intra-grain electronic quality and preventing the recombination activities at GBs/dislocations, or reduction of their presence altogether.

APPENDIX

2D-Device simulation in this work was performed using the electrical parameters listed in Table A-I and A-II. Hole and electron mobilities of LPC-Si were estimated as 80 % of the value of mono c-Si [2], [9]. In Table A-II, trap states of a-Si films were taken from standard a-Si layers compiled in AFORS-HET [21], [36], [37].

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Table A-I.

ELECTRICAL PARAMETERS USED IN DEVICE SIMULATION

	LPC-Si	a-Si(n)	a-Si(i)	a-Si(p)
Thickness (μm)	13	0.015	0.007	0.015
Electrical band gap (eV)	1.124	1.72	1.72	1.72
Electron affinity (eV)	4.05	3.9	3.9	3.9
Doping density (cm^{-3})	3/8/12 $\times 10^{16}$	7.5 $\times 10^{19}$	1 $\times 10^{13}$	7.5 $\times 10^{19}$
Electron mobility ($\text{cmV}^{-1}\text{s}^{-1}$)	747/620 /540	20	20	20
Hole mobility ($\text{cmV}^{-1}\text{s}^{-1}$)	311/266 /243	5	5	5

Table A-II.

TRAP STATES OF AMORPHOUS SI USED IN DEVICE SIMULATION

Films		a-Si (n)	a-Si (i)	a-Si (p)
Traps				
Conduction band tail	Total trap density ($\times 10^{19} \text{ cm}^{-3}$)	13.6	6.4	13.6
	Urbach energy (eV)	0.068	0.05	0.068
	e cross section ($\times 10^{-16} \text{ cm}^2$)	7	7	7
	h cross section ($\times 10^{-16} \text{ cm}^2$)	7	7	7
Valence band tail	Total trap density ($\times 10^{20} \text{ cm}^{-3}$)	1.88	9.4	1.88
	Urbach energy (eV)	0.068	0.035	0.068
	e cross section ($\times 10^{-16} \text{ cm}^2$)	7	7	7
	h cross section ($\times 10^{-16} \text{ cm}^2$)	7	7	7
Acceptor-like Gaussian defects	Energy peak from valence band (eV)	0.6	1.09	0.6
	Total trap density (cm^{-3})	7×10^{19}	5×10^{15}	7×10^{19}
	Correlation energy (eV)	0.21	0.144	0.21
	e cross section ($\times 10^{-15} \text{ cm}^2$)	3	3	3
	h cross section ($\times 10^{-14} \text{ cm}^2$)	3	3	3
Donor-like Gaussian defects	Energy peak from valence band (eV)	0.5	0.89	0.5
	Total trap density (cm^{-3})	7×10^{19}	5×10^{15}	7×10^{19}
	Correlation energy (eV)	0.21	0.144	0.21
	e cross section ($\times 10^{-14} \text{ cm}^2$)	3	3	3
	h cross section ($\times 10^{-15} \text{ cm}^2$)	3	3	3

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