The electrical properties of high performance multicrystalline silicon: Material limitation and cell potential

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Abstract — We compare the electrical properties of p-type and n-type industrial grown high performance multicrystalline silicon. The materials are characterised in terms of their bulk lifetimes, the density and recombination velocity of crystal defects, and their implied \(V_{OC}\). Quokka3 is applied to simulate the cell potential of the studied materials, and quantify the corresponding efficiency loss due to different recombination mechanisms occurring in the bulk. Our results show that bulk recombination in wafers from the middle of the ingot only contributes to negligible loss in conventional p-type Al-BSF solar cells. For higher efficiency solar cell structures, bulk recombination in HP mc-Si leads to a noticeable efficiency loss, varying from 0.6% to 1.6% absolute in the simulated devices, depending on the ingot position of the wafers. It is found that n-type HP mc-Si shows a slight advantage over p-type HP mc-Si, as it is less affected by recombination at the intra-grain regions.

I. INTRODUCTION

Multicrystalline silicon (mc-Si) is the most commonly used material for solar cell production [1]. The relatively low material cost of mc-Si has been the main contributor for its market dominance. In recent years, PV industries have started to employ high efficiency device architectures such as the passivated emitter and rear cell (PERC). These device structures have a higher requirement for the bulk material quality, which particularly presents a challenge for traditional mc-Si material. Mc-Si inherently contains crystal defects such as grain boundaries (GBs) and dislocations, and also relatively high metal impurity concentrations, originating from less pure crucibles and coatings. These act as recombination centres for carriers, and hence reduce the minority carrier lifetime.

There have been continuing efforts to improve the material quality of mc-Si. The most notable success is the recent development of the so-called high performance (HP) mc-Si material [2, 3], which has become the mainstream for mc-Si solar cell production. Compared to conventional mc-Si, HP mc-Si contains smaller grains, a large number of GBs and a lower number of dislocation clusters. It was found that the suppression of dislocation clusters in HP mc-Si, achieved by growing the ingot with smaller grains, significantly improves the final cell performance [2, 4].

Impurity control is another major concern for mc-Si materials [5, 6]. Various methods were developed to reduce metal impurity concentrations in mc-Si materials. These include using purer silicon feedstock, better contamination control in the crucibles and the silicon nitride coating, and growing larger ingots to minimise the contact fraction with the crucible walls. While these approaches combined have effectively reduced the overall metal impurity concentration in mc-Si ingots by more than one order of magnitude over the past decade [7, 8], it is argued that metal impurities in mc-Si can still lead to a significant efficiency loss, especially for high efficiency device designs [9]. N-type doping could be a solution to further improve the quality of mc-Si materials, given its higher tolerance to some commonly found metal impurities such as iron [10]. There have been numerous studies demonstrating the excellent electrical quality of n-type HP mc-Si [11-13]. The current record for mc-Si Si solar cells is based on n-type Si, namely the 22.3% n-type mc-Si TOPCon solar cell from Fraunhofer ISE [14]. In previous work [15], we reported average lifetimes up to 1.8ms for n-type HP mc-Si after boron, phosphorus diffusion and hydrogenation.

Mc-Si materials exhibit complex recombination behaviours. Previous works [9, 16-22] showed that wafers from different ingot positions exhibit distinct material properties, and their behaviours change substantially after cell processing steps. A comprehensive comparison between p-type and n-type HP mc-Si is relatively rare in the literature. In this work, we analyse the electrical properties of p-type and n-type industrial grown HP mc-Si, in terms of their as-grown properties, their ingot position dependence, their responses to cell fabrication, and their cell potential. The material quality is assessed based on their bulk lifetimes, the density and recombination velocity of crystal defects within the materials, and their implied \(V_{OC}\). The measured material properties are then correlated to cell performance modelled with Quokka3 [23]. Different bulk recombination losses in the materials are evaluated and compared quantitatively, to identify the key performance limiting factor of the materials. Rather than being limited to an arbitrary unit cell area, the modelling is performed on relatively large area (compared to the average grain size) mc-Si samples (> 4 cm × 4 cm) using measured photoluminescence (PL) images to realistically represent the inhomogeneous lifetime distributions in mc-Si materials.
II. EXPERIMENTAL METHODS

A. Sample Preparation

Wafers studied in this work were cut from different heights of central bricks from a G6 p-type boron doped HP mc-Si ingot and a G6 n-type phosphorus doped HP mc-Si ingot. The wafers were around 200 μm thick before any processing. P-type wafers were divided into groups and were subjected to various processing steps used in cell fabrication. Wafers from group A were as-grown controls. Wafers from group B went through texturing and phosphorus diffusion. The sheet resistance of the phosphorus diffusion was approximately 100 Ω/□. Wafers from group C went through texturing, phosphorus diffusion, and PECVD SiN deposition, and were then fired in a rapid thermal processing (RTP) furnace (Unitemp UTP-1100) for 10 s at 700 °C in N₂ ambient to produce bulk hydrogenation. N-type wafers received similar treatment as the p-type samples with an additional boron diffusion before the phosphorus diffusion.

For lifetime measurements, all wafers had the dielectric films and the heavily doped layers chemically removed, and were recoated with SiNx, on both the front and rear surfaces for passivation. Afterwards, all wafers were further treated for defect characterisation. The samples had the dielectric films removed, followed by SiN₃ deposition on their front surfaces, and thermal evaporation of thin metallic aluminum films (approximately 10 nm) on the rear surfaces. The aluminum films lead to instantaneous rear surface recombination conditions, which largely reduces the lateral carrier diffusion within the samples, thus allowing the crystal defects to be studied more accurately and independent of the properties of the intra-grain regions [24].

B. Lifetime characterisation

The lifetimes of the wafers were determined using a combination of quasi-steady-state photoconductance (QSSPC) lifetime measurements [25] using a WCT-120 tool from Sinton Instruments, and PL imaging [26] using the LIS-R1 tool from BT Imaging. The PL images were calibrated into absolute lifetime images based on an optically corrected calibration constant extracted from monocrystalline calibration wafers, described in detail in Ref. [27]. To investigate the intra-grain regions, pattern recognition algorithms were applied to the PL images to discriminate the intra-grain regions from the crystal defects, and the corresponding lifetimes were then extracted. A carrier de-smearing technique [28] was also applied to the calibrated lifetime images to account for the influence of lateral carrier smearing within the samples, to allow for a more accurate extraction of the intra-grain lifetimes.

C. Crystal defect characterisation

We applied a recently developed imaging technique [29] to evaluate the surface recombination velocity of extended crystal defects. The recombination properties of crystal defects were studied based on their spatial density and their surface recombination velocities (S_{defect}). The defect density was determined by applying pattern recognition methods to the PL images. S_{defect} values of individual defects were calculated based on their PL intensity contrasts and numerical modelling of the luminescence signal [24]. S_{defect} represents the intrinsic recombination properties of a defect and is independent of the lifetimes of the neighbouring regions surrounding the defect. The technique allows the overall recombination behaviours of crystal defects in a mc-Si wafer to be statistically quantified in an absolute scale, which enables a quantitative comparison of

Figure 1 – PL calibrated lifetime images of selected p-type HP mc-Si wafers before and after various processing. A logarithmic colour scale is used in the figure. The images were taken at 0.1 sun excitation conditions, corresponds to an injection level close maximum power point.
the recombination activities of crystal defects from different samples, before and after various processes.

D. Solar cell modelling

We applied 3D simulation to model the cell potential of the HP mc-Si materials studied in this work, and to quantify various recombination losses occurring in the Si bulk. The simulation is performed with Quokka3 [23], using artificially generated non-smeared lifetime images as inputs. The non-smeared images were created by combining injection dependent intra-grain lifetimes extracted from lifetime images taken at different excitation conditions and defect recombination velocity maps [29]. It was found that lateral carrier diffusion causes a smearing effect in the PL images, especially at high contrast features such as strongly recombination active GBs and dislocations. This smearing effect leads to a significant overestimation of the lifetimes at GBs and dislocations that cannot be fully corrected even with the proposed carrier de-smearing technique [28]. Schindler et al. [14] found that large-area Quokka3 simulation using de-smearing lifetime images does not reflect the actual cell performance accurately, and hence modelled the GB losses through single-grain simulation approach. To account for this, we used the intrinsic recombination velocity of a defect, extracted based on Ref. [24, 29], to determine a more accurate non-smeared lifetime at the defect. This allows us to perform large-area simulation to resolve bulk recombination losses in mc-Si.

III. RESULTS AND DISCUSSION

A. Material properties

Fig. 1 and 2 show lifetime images of p-type and n-type HP mc-Si from three ingot positions before and after boron diffusion (n-type only), phosphorus diffusion and hydrogenation (achieved through firing with SiN$_x$ films). While dislocation clusters remain recombination active regardless to the processing conditions, GBs show distinctive behaviours. Before any processing, GBs are only active in wafers from the top and bottom of the ingots, probably due to the higher metal impurity contamination in the wafers [8]. High temperature processing such as phosphorus or boron diffusion activates the GBs. However, most of the GBs can be passivated by subsequent hydrogenation treatment achieved through firing. The excellent hydrogenation effect of GBs is indeed the main reason for the superior performance of HP mc-Si in comparison to traditional mc-Si.

Fig. 3 compares the key material quality metrics of the studied p-type and n-type HP mc-Si. Apart from the top wafers, all other n-type samples show considerably higher average lifetimes compared to the p-type samples, owing to the significantly higher lifetimes in the intra-grain regions. The higher intra-grain lifetimes in the n-type samples could be due to the higher tolerance of metal contamination in n-type silicon [10]. In contrast, we do not observe any substantial variation in the recombination velocity of crystal defects between the p-type and n-type samples. This suggests the dominance of different recombination sources in the intra-grain regions and at crystal defects.

The influence of boron diffusion in n-type mc-Si is also worth noting, given that it is required to form the pn junction in n-type solar cells. It has been reported that the higher temperature used in boron diffusion can lead to thermal degradation in mc-Si [19, 30, 31]. Our results show that boron diffusion is mainly detrimental for crystal defects, except for the top wafers in which some intra-grain regions also degrade. Nevertheless, the negative impact of the boron diffusion can be effectively offset by subsequent phosphorus gettering and hydrogenation.

![Figure 2](image)

Figure 2 – PL calibrated lifetime images of selected n-type HP mc-Si wafers before and after various processing. A logarithmic colour scale is used in the figure. The images were taken at 0.1 sun excitation conditions, corresponds to an injection level close to maximum power point.
Both the p-type and n-type samples show very high implied $V_{oc}$ (≈ 720mV). Interestingly, although the n-type wafers show considerably higher lifetimes than the p-type wafers, their implied $V_{oc}$ turns out to be similar. This is due to the higher background doping in the p-type samples. This adds extra complexity when comparing p-type and n-type samples, in addition to their intrinsic difference in carrier mobility. In order to accurately compare the material quality of the studied samples, it is necessary to numerically model their cell efficiency.

![Graphs showing Harmonic average lifetime, Implied Voc from QSSPC, Average intra-grain lifetime, GBs and dislocation density, and Median S defects for p-type and n-type wafers](image)

Figure 3 – Summary of measured material properties for the studied p-type and n-type HP mc-Si wafers. Harmonic mean is used to represent the average lifetime. Implied $V_{oc}$ values were extracted from QSSPC measurements.

B. Cell modelling

We applied Quokka3 [23] to simulate the cell potential of the studied mc-Si wafers, and evaluate the efficiency loss caused by different bulk recombination mechanisms. For each studied wafer, four simulations were performed. The first simulation assumes only Auger recombination [32] occurs in the Si bulk, which provides the efficiency limitation for the chosen device structure. The second simulation uses the measured injection dependent intra-grain lifetime as input, which characterises the efficiency loss associated purely with recombination in the intra-grain regions. The third simulation uses the defect recombination velocity map [29] as input while assuming the intra-grain regions exhibit Auger lifetimes. It represents the efficiency loss associated purely with recombination at crystal defects. The fourth simulation uses the defect recombination velocity map [29] to approximate the lifetimes at crystal defects and uses the measured injection dependent intra-grain lifetimes for the intra-grain regions. It represents the efficiency loss induced by both bulk recombination channels (intra-grain regions and crystal defects), similar to an actual mc-Si solar cell in operation. All simulations were performed using parameters measured on diffused and hydrogenated wafers, as it reflects the material quality of samples after cell processing.

Fig. 4 shows the results of the simulation performed for p-type Al-BSF solar cells. Key parameters used in the simulation are listed in Table 1. Overall, bulk recombination (crystal defects and intra-grain regions) contribute to around 0.2% abs efficiency loss for middle wafers, and 0.4-0.5% abs efficiency loss for the top and bottom wafers. For top wafer, recombination at crystal defects dominates the total bulk recombination loss, due to the large density of dislocation clusters in the wafers, as shown in Fig. 1. For the bottom wafer, in addition to crystal defects, recombination at intra-grain regions contributes considerably to the overall efficiency loss. Moreover, our result suggests that the material quality of the middle wafers is sufficient for conventional Al-BSF solar cells, as the cell performance is more limited by other factors such as recombination at heavily doped regions or BSF regions at the rear.

![Graph showing efficiency and corresponding efficiency losses in p-type Al-BSF solar cells](image)

Figure 4 – Simulated cell efficiency and corresponding efficiency losses in p-type Al-BSF solar cells. The black bar refers to the Auger efficiency limitation of the chosen device structure. The red and blue bars correspond to efficiency loss associated with recombination at intra-grain regions or crystal defects respectively. The pink bar refers to efficiency loss due to the combined influences of recombination at intra-grain regions and crystal defects.

Fig. 5 shows the simulation results when applied on high efficiency solar cell structures. Simulations for p-type mc-Si are based on a PERC structure with black silicon texturing and selective front doping. Device parameters are estimated based on reported record cell efficiency for mc-Si solar cells and best achievable industrial parameters (screen printed large area
For the n-type bi-facial doped-poly solar cell, bulk recombination (crystal defects and intra-grain regions) contribute to around 0.8% abs efficiency loss for middle wafers, and 1.3 - 1.6% abs efficiency loss for the top and bottom wafers. Note that the two simulated cells (p-type and n-type) feature different cell structures, and hence show different intrinsic efficiency (21.9% for the p-type PERC and 22.3% for the n-type bi-facial doped-poly structures). Compared to the p-type samples, we observed a slightly higher recombination loss due to crystal defects in the n-type samples, owing to the slightly higher density of crystal defects, as shown in Fig. 3. Since dislocation clusters exist non-uniformly among mc-Si wafers, the small difference could be due to sample-to-sample variation, rather than any actual physical difference in the density of crystal defects in p- and n-type ingots, which in principle would not be expected. More work is needed to verify these findings.

Interestingly, in the studied n-type samples, bulk recombination loss is dominated by recombination at GBs and dislocations, whereas only a small percentage of loss is through recombination at intra-grain regions. N-type HP mc-Si might therefore retain a slight advantage over p-type HP mc-Si, as it is relatively unaffected by intra-grain recombination. However, the difference is not large, and can be overshadowed by other factors. Nevertheless, both p-type and n-type HP mc-Si from the middle of the ingot show simulated cell efficiencies well above 21%, demonstrating the potential for both materials to be used for high efficiency devices in mass production.

Note that the simulated cell efficiencies are sensitive to the device architectures and depend strongly on the parameters used in the modelling. The reported values only provide an approximate indication of the efficiency losses due to bulk recombination. Nevertheless, our estimated efficiency losses caused by recombination at crystals defects in the middle wafers are similar to the reported values by Schindler et al. [14] for their 22.3% TOPCon solar cell (0.7% abs from Ref. [14] and 0.6% abs in this work), despite the different material and device parameters used in the two simulations. Moreover, Needleman et al. [33] applied Technology Computer Aided Design (TCAD) modelling to simulate the efficiency loss caused by dislocations in a 21.25% p-type PERC solar cell. The reported values (0.26% abs) are also comparable with those determined in this work (0.18% abs).

IV. CAST MONO-LIKE SILICON

Mono-like silicon is an alternative cast-grown material for PV production. The material is cast using a seeding layer consisting of monocrystalline silicon slabs of specific orientation to control the growth direction. It contains a significantly reduced number of GBs, and more importantly, can be grown with mostly (100) surface orientation, making it compatible with the alkaline texturing commonly used on Czochralski-grown (Cz) silicon. Mono-like silicon has attracted great attention in PV industries, although it was found that the material often suffers from a low ingot yield due to the propagation of dislocation networks towards the top of the ingot. Material analysis on both p-type and n-type mono-like silicon will be included in upcoming work.
Table 1 - A list of some of the main parameters used in the simulations.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>P-type Al-BSF</th>
<th>P-type PERC</th>
<th>N-type bi-facial doped-poly</th>
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<tr>
<td>Optical generation current</td>
<td>mA/cm²</td>
<td>Value</td>
<td>Value</td>
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<td>42</td>
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<td></td>
<td>50</td>
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<tr>
<td>Jo for contacted regions</td>
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<td>1000</td>
<td>850</td>
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<tr>
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<td>150</td>
<td>20</td>
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<tr>
<td>Jo for heavily doped region</td>
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<td>40</td>
</tr>
<tr>
<td>Rear</td>
<td></td>
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<tr>
<td>Jo for contacted regions</td>
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<td>300</td>
<td>600</td>
</tr>
<tr>
<td>Jo for passivated regions</td>
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<td>15</td>
<td>13.1 [37]</td>
</tr>
<tr>
<td>Contact resistivity</td>
<td>mohm-cm²</td>
<td>20</td>
<td>5</td>
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</table>

V. CONCLUSION

We have performed a direct comparison of the electrical properties and cell potential of p-type and n-type industrial grown HP mc-Si. It is found that the material properties change substantially after cell processing steps, indicating the importance of considering such effects when evaluating mc-Si. While the bulk quality of HP mc-Si wafers from the middle of the ingot appears to be good enough for conventional Al-BSF, recombination at intra-grain regions and crystal defects still leads to a certain extent of efficiency loss in higher efficiency devices. Nevertheless, both the p-type and n-type HP mc-Si materials show simulated cell potential well above 21%, based on a p-type PERC and an n-type bi-facial doped-poly cell structure. The small apparent advantage of n-type HP mc-Si over p-type HP mc-Si mainly comes from the higher lifetimes in the intra-grain regions, although the difference is not large.

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REFERENCES


