3-D Modeling of Multicrystalline Silicon Materials and Solar Cells


Abstract—We present a method to model large-area multicrystalline materials using Quokka3, based on artificially generated lifetime images created by combining injection-dependent intra-grain lifetimes and defect recombination velocity maps extracted from photoluminescence-based lifetime images. It is found that simulations based only on measured lifetime images underestimate the detrimental impacts of crystal defects and, hence, overestimate the overall cell performance of multicrystalline silicon solar cells. As demonstration, we applied Quokka3 simulations to resolve various bulk recombination losses in industrial multicrystalline silicon solar cells, quantify the effects of phosphorus diffusion and hydrogenation on the final cell performance, and evaluate the detrimental impact of crystal defects on individual cell parameters. Through numerical simulations, this paper has also demonstrated the potential errors of using a single average value to predict the cell performance of inhomogeneous multicrystalline silicon materials. It is observed that the commonly used harmonic mean can provide a good indication for $V_{oc}$, but is less effective for predicting $J_{sc}$, and is almost entirely ineffective for predicting the fill factor.

Index Terms—Grain boundaries, impurities, photoluminescence, semiconductor device modeling, silicon.

I. INTRODUCTION

UNDERSTANDING bulk recombination mechanisms in multicrystalline silicon (mc-Si) is crucial to determine its potential and limitations for solar cell applications. mc-Si materials exhibit complex recombination behaviors. Wafers from different ingot positions show distinct material properties, in terms of their as-grown properties and their responses to cell processing steps [1]–[8], primarily due to the presence of crystal defects such as grain boundaries (GBs) and dislocations in the materials, and their interactions with metal impurity contamination and thermal processes. These localized GBs and dislocations also introduce strongly inhomogeneous lifetime distributions in mc-Si wafers, which pose a challenge for characterization and simulation. An empirical approach is often used to study mc-Si in the photovoltaic industry, via correlating material properties measured on ingots or wafers with their final cell performance [9]–[12]. One example is the work of Mitchell et al. [10], who correlated as-grown material quality with the performance of passivated emitter and rear cell (PERC) solar cells and suggested the use of dislocation density as a performance predictor for mc-Si solar cells. These approaches are straightforward, and the large amount of data available in production lines allow the analysis to be statistically significant. However, such analysis can only provide limited physical insight into the materials and, more importantly, depends heavily on the cell production lines and the materials themselves and, hence, is more suited for quality monitoring or wafer sorting.

Numerical simulations can be applied to model mc-Si devices. The development of spatially resolved measurement techniques such as photoluminescence (PL) imaging [13], electroluminescence (EL) imaging [14], and dark lock-in thermography (DLIT) [15] has allowed the local material properties of mc-Si to be measured and used as inputs for numerical modeling. One commonly used approach to model inhomogeneous mc-Si devices is by treating it as a network of individual solar cells connected in parallel [16]–[20]. Michl et al. [18] developed the efficiency-limiting bulk recombination analysis method, which uses a one-dimensional device modeling tool to model the $I$–$V$ characteristics of individual components of solar cells based on calibrated PL lifetime images, combined with SPICE circuit simulations to model the lateral current flow and the global cell performance. Similar approaches were implemented in commercial simulation packages such as Griddler [21], [22]. The key advantage of these multiscale simulation approaches is that they eliminate the need to perform three-dimensional (3-D) simulation, which can be computationally expensive, and hence, they can be applied to model large-area mc-Si devices. However, it can be argued that such circuit simulations do not fully account for the influence of lateral or diagonal carrier transport occurring within the Si bulk.
Commercial device simulators like Synopsys Sentaurus Device [23] can be used to model multidimensional semiconductor devices without major simplifications. Altermatt et al. [24] applied Sentaurus Device to simulate lateral current flow in mc-Si using a two-dimensional (2-D) model. Needleman et al. [25], [26] extended the model to investigate the detrimental impact of GBs and dislocations in a 3-D mc-Si device, incorporating the effect of charging associated with the defects. Such detailed simulations are accurate, but, due to computational complexity, are often limited to 2-D projections or a single 3-D unit cell, which might not be representative of a large-area mc-Si device, particularly for locally distributed dislocation clusters.

In this paper, we demonstrate a method to model large-area mc-Si materials in 3-D using Quokka3 [27]. By applying the conductive boundary approach [28], [29] and assuming bulk quasi-neutrality, Quokka3 largely reduces the computation effort to simulate carrier transport in solar cells, making it possible to solve large 3-D geometries within manageable timeframes for modeling full-area mc-Si devices. Schindler et al. [30] applied Quokka3 to analyze efficiency loss mechanisms in 2 cm × 2 cm n-type HP mc-Si solar cells and found that large-area Quokka3 simulations based on PL-derived lifetime images do not reflect the actual cell performance accurately, which they attribute to the pixel resolution of the PL camera, and electrical and optical smearing effects in the PL images [31], [32]. Here, we demonstrate the use of artificially generated nonsmeared lifetime images, created by combining injection-dependent intragrain lifetimes extracted from PL-derived lifetime images and defect recombination velocity maps [33], as input for Quokka3, to accurately resolve bulk recombination losses in large-area (> 4 cm × 4 cm) mc-Si solar cells. As shown in detail below, it is crucial to use nonsmeared lifetime images to properly simulate the lateral carrier transport in a solar cell device, to avoid double counting of the lateral smearing effect. Moreover, the degree of carrier smearing in a PL image is also very different to the degree of carrier smearing in a device with heavily doped layers under different operation conditions. This paper will discuss several application examples for performing such large-area simulations on mc-Si materials, aiming to answer some commonly discussed questions concerning mc-Si characterization, including the detrimental impact of crystal defects, the benefit of phosphorus gettering and hydrogenation, and the uncertainty in using average lifetimes to represent mc-Si materials.

II. METHODS

A. Method Description

Given its rapid, nondestructive, and contactless nature, the PL imaging technique is well suited for measuring local lifetime properties of mc-Si for numerical modeling. However, PL images suffer from a “smearing” effect due to lateral carrier diffusion [32], especially at high contrast features such as strongly recombination active GBs and dislocations. This leads to a significant overestimation of the lifetimes at GBs and dislocations, and an underestimation at nearby regions. This cannot be fully corrected, even when using “desmeared” images created from numerical carrier desmearing techniques [32], [34], resulting in errors when the images are used as inputs for simulations.

![Fig. 1. (a) $S_{\text{defect}}$ map for a phosphorus-gettered HP mc-Si wafer from the middle of an ingot. (b) Nonsmeared. (c) smeared, and (d) desmeared lifetime images of a simulated mc-Si wafer. (d) Cross-sectional profile of the simulated wafer across the highlighted line in (b). The images are derived based on a phosphorus-gettered HP mc-Si wafer from the middle of an ingot.](image)

To account for this effect, we use artificially generated lifetime images as inputs for Quokka3 simulations, which we call “nonsmeared” images. The nonsmeared images were created by combining injection-dependent intragrain lifetimes extracted from lifetime images taken at different excitation conditions and defect recombination velocity maps [33]. Samples used for intragrain lifetime extraction were well passivated with SiNx on both the front and rear surfaces. Pattern recognition algorithms were applied to the PL images to discriminate the intragrain regions from the crystal defects, and the corresponding lifetimes were then extracted after applying carrier desmearing [32], [34]. Samples used for defect characterization received SiNx on their front surfaces and thin aluminum films on their rear, to achieve instantaneous surface recombination conditions at rear, to achieve instantaneous surface recombination conditions at rear, which allows the extraction of the surface recombination velocity of extended crystal defects such as GBs and dislocations ($S_{\text{defect}}$), as described in detail in [33] and [35]. $S_{\text{defect}}$ values of
individual defects were calculated based on their PL intensity contrasts and numerical modeling of the luminescence signal [35], accounting for both the lateral carrier diffusion within the bulk and the pixel size of the PL camera. We then used the intrinsic recombination velocity of a defect to determine a more accurate nonsmeared lifetime at the defect. An example of the defect recombination velocity map is shown in Fig. 1(a), for a phosphorus-gettered HP mc-Si wafer from the middle of an ingot.

Fig. 1 compares nonsmeared, smeared, and desmeared lifetime images of a simulated mc-Si wafer featuring a certain number of strongly recombination active GBs, to demonstrate the importance of considering this later carrier smearing effect in numerical simulations. We first derive a nonsmeared lifetime image in Fig. 1(b) based on the defect recombination velocity map shown in Fig 1(a) and then numerically simulate the lateral carrier diffusion, assuming 1-sun open-circuit condition, to obtain the smeared lifetime image in Fig. 1(c). Afterward, we applied a carrier desmearing method based on the continuity equation [32], [34] to correct for the lateral carrier diffusion and generate the desmeared lifetime image in Fig. 1(d). For model simplification, an injection-independent intragrain lifetime of 300 µs is assumed in these simulations. Measurement noise is added in Fig. 1(c) to better represent actual PL measurements. The line-scan profile in Fig. 1(e) shows that lateral carrier diffusion significantly reduces the overall signal contrast. While the application of carrier desmearing recovers the lifetimes in the intragrain regions, it is not fully effective around strongly recombination active features. More than an order of magnitude overestimation in lifetimes at GBs and dislocations can still be present in the desmeared lifetime image. Shown also in the lifetime images (see Fig. 1) are the Quokka3 simulated performance of a PERC solar cell based on each lifetime image. It can be observed that the overestimation of lifetimes at GBs and dislocations in the smeared or even the desmeared lifetime images leads to an overestimation in the simulated device performance, resulting in a strong underestimation of the detrimental impact of GBs and dislocations.

Note that the errors introduced by this lateral carrier smearing effect are not related to the simulation software, but rather due to the inaccurate input images used for the simulation, owing to the overestimation of lifetimes at GBs and dislocations in the input images. Furthermore, this lateral smearing effect is not only limited to PL imaging techniques, but also applicable to other measurement techniques such as EL and DLIT.

In addition to carrier smearing, PL images are also affected by optical smearing phenomenon in the silicon charge-coupled device sensor [31]. In this paper, a short-pass filter with a cutoff wavelength of 1050 nm was fitted in the imaging lens to reduce the impact of such effect in the acquired PL images. Image deconvolution using an experimentally determined point spread function was also applied to the PL images to further eliminate its remaining influence [36].

Moreover, it should be noted that the “sharpness” of any lifetime image is fundamentally limited by its pixel resolution. The nonsmeared lifetime image in Fig. 1(b) is derived by integrating a defect recombination velocity map in Fig 1(a) over a certain pixel size (162 µm in this paper) and, hence, only provides an approximation for the actual interface recombination at crystal defects. To investigate this uncertainty, we performed a single grain simulation, which models GB as a vertical recombining surface ($S_{\text{defect}} = 10000 \text{ cm/s}$), and compared the result with the simulation based on the corresponding lifetime image with a pixel size of 162 µm. An error of less than 0.1% absolute is observed between the two simulation approaches, for a PERC solar cell with efficiency around 21%. Furthermore, the simulation result is also affected by the mesh size used in the finite-element simulation. We have used a maximum mesh size of 300 µm in the finite-element grid in this paper, balancing between simulation accuracy and computation time.

B. Method Verification

For verification, we applied the proposed method to model solar cell performance along an mc-Si ingot based on lifetime samples and compared it with the performance of actual solar cells fabricated using sister wafers. The mc-Si wafers studied here were cut from different heights of a central brick of a G6 industrially grown p-type boron-doped HP mc-Si ingot. Sister wafers from each position were divided into two groups. Wafers from the first group were fabricated into Al-back surface field (Al-BSF) solar cells in an industrial production line. The cell process involves texturing, POCl₃ diffusion, plasma enhanced chemical vapor deposition SiNₓ deposition, front and back screen-print metallization, and metallization firing. Wafers from the second group were subjected to the similar treatment as the first group, but fired in a belt furnace without the metallization paste. The wafers were then cut into smaller pieces (5 cm × 5 cm), chemically etched to remove any surface films and n⁺ layers, and recoated with SiNₓ and/or aluminum films to produce nonsmeared lifetime images used for Quokka3 modeling. The SiNₓ films used for repassivation provide excellent surface passivation with $S_{\text{eff}}$ below 10 cm⁻³ (confirmed with monocrystalline silicon control wafers), while having a low deposition temperature ($\approx 300°C$) to minimize further bulk hydrogenation occurring during the deposition.

We used the same device parameters (Optics, $J_0$, contact resistivity, etc., as shown in Table I) in the simulations so that any observed differences in the simulated efficiencies among the studied samples are solely a bulk effect, including the influence of resistivity variation along the ingot. The device parameters selected based on previous literature and, then, adjusted to obtain the best fit between the simulated and measured values. Fig. 2 shows that our simulated cell efficiencies match well with the actual cell performance, including wafers toward the top and the bottom of the ingot, where their efficiencies suffer from their lower material qualities, indicating the validity of our method. The individual cell parameters also agree reasonably well with the simulated values. The small discrepancy may be due to imprecise device parameters used in the simulation, uncertainty in the intragrain lifetime extraction, imperfect pattern recognition algorithms used to detect or differentiate crystal defects and intragrain regions, property variations within a 15.6 cm × 15.6 cm mc-Si wafer (the modeling is based on a
TABLE I  
LIST OF SOME OF THE MAIN PARAMETERS USED IN THE SIMULATIONS

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Unit</th>
<th>Value</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optical generation current</td>
<td>mA/cm²</td>
<td>39.1</td>
<td>37.9 – 39.1[41]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>37.3 – 38.8[42]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>41</td>
<td>Approximated based on Ref. [43]</td>
</tr>
<tr>
<td>Sheet resistance for lightly doped region</td>
<td>ohm</td>
<td>90</td>
<td>70 – 90 [44]</td>
</tr>
<tr>
<td>Sheet resistance for heavily doped region</td>
<td></td>
<td>150</td>
<td>90-160 [44]</td>
</tr>
<tr>
<td>J₀ for contacted regions</td>
<td>fA/cm²</td>
<td>1400</td>
<td>1800 [45]</td>
</tr>
<tr>
<td>J₀ for lightly doped region</td>
<td>fA/cm²</td>
<td>65</td>
<td>100 – 200 [46]</td>
</tr>
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<td>fA/cm²</td>
<td>8</td>
<td>100 – 200 [46]</td>
</tr>
<tr>
<td>Contact resistivity</td>
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<td>300 – 700 [44]</td>
<td>450</td>
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<td>J₀ for passivated regions</td>
<td>fA/cm²</td>
<td>15</td>
<td>13.1 [44]</td>
</tr>
<tr>
<td>Contact resistivity</td>
<td>mohm·cm²</td>
<td>8</td>
<td>5 [44]</td>
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</table>

Fig. 2. Actual and simulated (a) cell efficiency, (b) $V_{oc}$, (c) $J_{sc}$, and (d) FF for Al-BSF solar cells from different heights of a p-type HP mc-Si ingot. The right y-axis shows the variation (in percent) in the data, normalized based on the mean value in the left y-axis. Main parameters used in the simulations are listed in Table I.
5 cm × 5 cm region within the sample), and injection-dependent recombination velocities of crystal defects, which have not been accounted for in the extraction of $S_{\text{defects}}$. A slightly larger discrepancy is observed in fill factor (FF) for samples toward the ingot bottom. This could be attributed to the small grain size in these samples, which increases the uncertainty in the intragrain lifetime extraction especially at low injection levels, where the signal-to-noise ratio is low, affecting the injection dependence of the intragrain lifetimes used in the simulations.

### III. Application Examples

#### A. Bulk Recombination Loss Analysis

Large-area 3-D modeling can be used to quantify bulk recombination loss in mc-Si solar cells. To demonstrate this, we applied Quokka3 to evaluate the efficiency loss due to recombination at crystal defects and intragrain regions in Al-BSF and PERC solar cells made from p-type HP mc-Si wafers from different ingot heights. For each studied wafer, four simulations were performed. The first simulation assumes that only intrinsic (Auger [37] and radiative) recombination occurs in the Si bulk, which provides the efficiency limitation for the chosen device structure. The second simulation uses the measured injection-dependent intragrain lifetime as input, which characterizes the efficiency loss associated purely with recombination in the intragrain regions. The third simulation uses the defect recombination velocity map [33] as input, while assuming that the intragrain 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 [33] to approximate the lifetimes at crystal defects combined used the measured injection-dependent intragrain lifetimes for the intragrain regions. It represents the efficiency loss induced by both bulk recombination channels (intragrain regions and crystal defects), similar to an actual mc-Si solar cell in operation.

All simulations were performed using bulk parameters measured on diffused and hydrogenated wafers, as it reflects the material quality of samples after cell processing. The injection-dependent intragrain lifetimes were extracted from PL images taken at different excitation conditions. The local nonsmeared lifetimes at crystal defects were calculated from the corresponding defect recombination velocity maps [33], where the $S_{\text{defect}}$ values of individual defects were determined based on their PL intensity contrasts and numerical modeling of the luminescence signal [35].

Fig. 3(a) shows the results of the simulation performed for p-type Al-BSF solar cells. Key device parameters used in the simulation are listed in the Table I. Overall, bulk recombination (crystal defects and intragrain regions) contributes to around 0.2% absolute efficiency loss for middle wafers and around 0.4% absolute efficiency loss for the top and bottom wafers. For top wafers, recombination at crystal defects dominates the total bulk recombination loss, owing to the large density of dislocation clusters in those wafers and their strong recombination behaviors, possibly due to the heavy decoration of metal impurities as a result of the high metal impurity concentration toward the top of the ingot. This suggests that the propagation of dislocation networks continues to be a key performance-limiting factor for HP mc-Si wafers toward the ingot top. For the bottom wafers, in addition to crystal defects, recombination in the intragrain regions contributes considerably to the overall efficiency loss. Moreover, the simulated efficiency for wafers from the middle of the ingot approaches the device limit, suggesting that its cell performance is more limited by other factors such as recombination at the heavily doped regions or the surfaces.

Fig. 3(b) shows the simulation results when applied on a high-efficiency solar cell structure. Simulations are based on a PERC structure with black silicon texturing and selective front doping. Device parameters are estimated based on reported record cell efficiencies for mc-Si solar cells and the best achievable industrial parameters (screen-printed large-area solar cells). The main parameters used in the simulations are listed in the Table I.
The overall behaviors of PERC solar cells are similar to the Al-BSF, except that the final cell performance is more sensitive to the bulk properties owing to their higher efficiency. Bulk recombination (crystal defects and intragrain regions) contributes to around 0.6% absolute efficiency loss for the middle wafers and 1.2–1.3% absolute efficiency loss for the top and bottom wafers. In particular, crystal defects solely contribute to a 1.0% absolute efficiency loss for wafers toward the ingot top.

B. Quantifying the Influence of Thermal Processes

Quokka3 modeling can also be used to evaluate the influence of thermal processes on the performance of mc-Si solar cells. Phosphorus gettering and hydrogenation are incorporated in common solar cell fabrication steps during the formation of p-n junctions and firing of metal contacts. While there are many works [2], [5], [6] showing the benefits of phosphorus diffusion in improving the intragrain lifetimes via gettering metal impurities from the Si bulk, it is less clear whether its overall impact on cell performance is positive given that the high temperature used in the process also increases the recombination activities of crystal defects [1], [5], [6]. As an example, Fig. 4(a) shows the lifetime and defect properties of a p-type HP mc-Si wafer from the middle of an ingot before and after phosphorus gettering and hydrogenation. The overall lifetime, as represented by the harmonic mean, reduces after phosphorus gettering despite the improvement in the intragrain lifetimes. We applied Quokka3 to model the potential cell efficiency of this particular sample before and after thermal processes, using measured injection-dependent intragrain lifetimes and the corresponding defect recombination velocity maps [33]. The result is shown in Fig. 4(b). Our result shows that phosphorus gettering alone is actually detrimental to the cell efficiency in the studied wafer as the activation of GBs introduces substantial recombination losses, increasing from 0.5% to 1.8% absolute. On the other hand, subsequent hydrogenation is very effective in passivating GBs, significantly reducing their impact on the final cell efficiency.

Note that wafers cut from different ingot heights feature different bulk properties, hence, can respond differently to gettering and hydrogenation. For instance, it is found that the benefit of gettering in the intragrain regions outweighs its negative impact on crystal defects in wafers toward the very top and bottom of the ingot, due to the fact that crystal defects in those samples are already very recombination active in the as-grown state. A comprehensive study of the material properties of HP mc-Si ingot will be included in future work.

C. Impact of Crystal Defects on Individual Cell Parameters

We model a range of mc-Si samples cut from different ingot heights, before and after various processing steps (as-grown, gettered, and hydrogenated), making use of these samples featuring different density, spatial distribution, and recombination behaviors of crystal defects to study the detrimental impact of crystal defects on individual cell parameters. An injection-independent intragrain lifetime of 300 µs is assumed in all samples for model simplification and to eliminate its influence on the simulations.

Fig. 4. (a) Lifetimes and defect properties of a p-type HP mc-Si wafer from the middle of an ingot before and after phosphorus gettering and hydrogenation. Lifetimes were extracted at 0.1-sun excitation conditions. Harmonic mean is used to represent the average lifetime. The product of the defect density and their median $S_{\text{defects}}$ value is used to represent the overall recombination activities of crystal defects in the sample. (b) Simulated potential cell efficiency and corresponding efficiency losses for the p-type HP mc-Si wafer before and after gettering and hydrogenation. 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 intragrain regions or crystal defects, respectively. The pink bar refers to efficiency loss due to the combined influences of recombination at intragrain regions and crystal defects. P denotes phosphorus-gettered samples, whereas P+H denotes phosphorus-gettered and hydrogenated samples.

Fig. 5 shows the correlation between the defect product in the samples, which is defined as the product of the defect density and their median $S_{\text{defects}}$ value, and the corresponding cell performance simulated with Quokka3. Here, we have chosen to use the defect product to represent the overall recombination behaviors of crystal defects in the studied samples, accounting for both the density of crystal defects and their recombination strength. Recombination at crystal defects affects all cell performance parameters ($V_{\text{oc}}$, $J_{\text{sc}}$, and FF), but is most detrimental to the $V_{\text{oc}}$. Recombination at crystal defects leads to local reductions of lifetime and excess carrier concentration at the defects, resulting in a local reduction of both the open-circuit voltage and the short-circuit current. Surprisingly, a reduction in the FF can also be observed with increasing density or recombination...
activities of crystal defects. This is not caused by injection-dependent lifetime properties of the intragrain regions or at the defects, as both of them are assumed to be injection independent in this simulation. The reduction of the FF is likely to be caused by an increase in lateral carrier diffusion via the heavily diffused regions at the maximum power point (MPP) compared with open-circuit conditions, due to the lower injection level at the MPP, which extends the spatial influence of crystal defects further into the adjacent grains, which has also been found in [30]. Moreover, it is anticipated that the injection-dependent recombination properties of the defects [38] and at intragrain regions [6] should lead to an even larger FF loss in an actual mc-Si cell.

It is noted that the samples used in this simulation are from different ingot positions. Wafers from ingot bottom contain more GBs, which tend to be dispersed, whereas wafers from ingot top contain more dislocation clusters, which are generally highly localized. The spatial distribution of crystal defects can impact the cell performance, and this is partly reflected in the nonstrictly monotonous relationship shown in Fig. 5.

D. Averaging Methods for Representing mc-Si

As shown above, 3-D mc-Si simulation based on lifetime images is very effective for modeling the performance of mc-Si solar cells. However, such modeling can still be too time-consuming to be used for routine analysis. Hence, it is often valuable to use a single spatially averaged lifetime value or an injection-dependent lifetime curve (derived using spatially averaged lifetimes extracted from lifetime images taken at different excitation conditions) to evaluate mc-Si material and to predict its cell performance. Choosing an appropriate mean to represent inhomogeneous mc-Si materials is not trivial. The generalized mean for a set of positive number can be defined as

\[
M_p (x_1, \ldots, x_n) = \left( \frac{1}{n} \sum_{i=1}^{n} x_i^p \right)^{1/p}
\]  

(1)

where \( p \) defines the types of mean obtained. Two commonly used means for mc-Si characterization are the arithmetic mean \((p = 1)\) and the harmonic mean \((p = -1)\), which are derived based on the additive lifetimes and the recombination rate, respectively [39].

We compare the efficiencies of mc-Si solar cells simulated based on inhomogeneous nonsmeared lifetime images of mc-Si wafers such as Fig. 1(b) and the ones simulated using homogeneous average lifetime values calculated from the corresponding smeared lifetime maps such as Fig. 1(c), using different \( p \) values according to (1). Wafers from different ingot heights and at various processing steps were used in this comparison to evaluate the impacts of crystal defects on the averaging method. For model simplification, an injection-independent intragrain lifetime of 300 \( \mu s \) is assumed in all samples instead of the measured intragrain lifetimes. The same doping concentration \((1 \times 10^{16} \text{ cm}^{-3})\) is assumed on all samples.

Fig. 6(a) shows that the harmonic mean provides a closer approximation to the cell efficiency when compared with the arithmetic mean, as it is more influenced by the lower lifetime regions in mc-Si, but still overestimates the cell efficiency particularly on wafers with high density of crystal defects. It is found that mean values with \( p = -1.5 \) produce the best approximation to the final cell efficiency for the samples studied in this paper. Our optimal \( p \) value is smaller than that reported by Wagner et al. [19] \((p \approx -0.75)\). This is mainly due to the fact that the mean values here are calculated based on smeared lifetime images, analogous to typical PL measurement conditions, whereas the values calculated in [19] are based on nonsmeared lifetime maps.

Fig. 6(b) and (c) shows the uncertainties of using global means to predict individual cells parameters. Surprisingly, it is observed that harmonic average \((p = -1)\) can provide a very good indication for \( V_{oc} \), while being only somewhat effective for predicting \( J_{sc} \), and is almost ineffective for predicting the FF. \( J_{sc} \) can be best predicted using a mean calculated with a \( p \) value of \(-1.5\), whereas no \( p \) value can accurately predict the FF. This discrepancy is mainly due to the fact that the detrimental impacts of crystal defects are weighted differently on \( V_{oc} \), \( J_{sc} \), and FF, as observed in Fig. 5, being affected by factors such as the injection levels, the extent of lateral carrier diffusion, and carrier collections [19], [39], [40], coupled with the individual nonlinear relationships between bulk lifetime and cell parameters. Our results suggest that it might be more accurate to use different global means to predict \( V_{oc} \), \( J_{sc} \), and FF, separately, and combine them afterward to model the overall efficiency.

It is noted that the correlation shown in Fig. 6 is solely an empirical correlation derived based on the p-type PERC HP mc-Si solar cells studied in this paper. The optimal averaging method can vary depending on the cell structures, material properties, lifetime distribution, pixel resolution of PL images,
Fig. 6. Comparison in (a) efficiency, (b) $V_{oc}$, (c) $J_{sc}$, and (d) FF between modeling based on inhomogeneous lifetime maps and modeling using a single average lifetime value calculated from the corresponding lifetime maps. Different values of $p$ are used to calculate the average lifetimes according to (1). The diagonal line represents zero variation between the two simulation approaches. Data point above this line corresponds to an overestimation in the simulated efficiency in the averaging approach, and vice versa.

and measurement conditions (open circuit, short circuit, etc.). Fundamentally, only the harmonic mean derived based on the additive of recombination rate contains physical meaning; any other $p$ values are a numerical compensation of the model simplifications. It is important to consider the potential errors of using a single mathematical average to evaluate and compare mc-Si materials.

IV. CONCLUSION

We have presented a method to model large-area mc-Si materials in 3-D using Quokka3, based on artificially generated nonsmeared lifetime images created by combining injection-dependent intragrain lifetimes extracted from lifetime images and defect recombination velocity maps. We have applied the modeling to quantify different bulk recombination activities in mc-Si materials and their interaction with thermal processes. Our results confirm that recombination at crystal defects plays a very important role in the performance of mc-Si devices. Phosphorus diffusion is not necessarily beneficial to mc-Si materials, as it also activates GBs and dislocations. Moreover, it has been found that the commonly used harmonic mean provides a closer approximation to the cell efficiency when compared with the arithmetic mean, but still overestimates the cell efficiency particularly on wafers with high density of crystal defects.