Statistical insights from inline solar cell metrology data in a PERC production environment

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Abstract

The adaptation of solar cell physics models and advanced laboratory-based measurement techniques to enable their use in high-volume, inline solar cell production settings is an exciting development towards implementing Industry 4.0 compliant smart solar cell factories. This paper outlines how a blend of physics-based analysis and statistical data science methods can aid continuous improvement and yield optimization in high-volume solar cell fabrication. A specific example is provided for a passivated emitter, rear locally contacted (PERC) solar cell production environment, where four batches of 500 commercial solar cells are evaluated using *I–V* at one-Sun as well as both contacted and contactless spectral response techniques. The spectral response techniques revealed prominent periodic patterns in the cell measurement sequence, which could be traced to the anti-reflection coating deposition process. This process inhomogeneity led to bimodal distributions in each batch with an efficiency difference as large as 0.07% between the modes. Thus, its identification by the spectral response technique is an important first step towards improving the efficiency distribution via deposition uniformity improvement. A yield-oriented cell physics model is used to interpret the various data in the context of underlying cell parameters, forming the basis for previously impractical root cause analysis in complex adverse events, and for process optimization in order to obtain sustained yield improvement in high-volume production.

Introduction

While the solar industry is undergoing unprecedented levels of capacity expansion – exceeding 500GW across ingot/wafer, solar cell and module assembly segments combined in the first quarter of 2020 [1], the rate at which world electricity sources are transitioning from fossil fuel to renewable energy must further *increase* for the world to ward off disastrous levels of global warming [2]. For PV to do its part, terawatt levels of production will soon be required, and advanced manufacturing concepts must therefore be successfully implemented to support these new volumes of production.

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The Industry 4.0 framework, which originated in 2011, outlines a number of timely and important concepts that address the need for greater levels of digitization and data analytics as manufacturing continues to scale up. One of these important concepts is the *digital twin*, a near-real-time digital image of a physical object or process that helps optimize business performance [3]. When applied to solar cell manufacturing, a digital twin can be considered to be akin to solar cell device models and fabrication process simulations [4–5]. This opens up the field for analytical modelling, simulation and optimizations that converge to derive value from massive volumes of data, leading to significant improvements in cost and process efficiencies [5].

Just as the brain applies a cognitive model of the world on sensory data, a digital twin is effective only if it is fed a continuous, rich set of measurement data derived from the operation of manufacturing processes. In this context, recent trends in solar cell factories point towards an increasing richness of end-of-line measurement data on the finished device, with electroluminescence (EL) and infrared (IR) imaging becoming standard, while the *I–V* tester has also gone through innovations that enable it to measure more than just the current–voltage characteristics [6–7]. One of the most exciting developments is the advent of *I–V* testers with monochromatic LED illumination that have tuneable spectra and therefore the capability of measuring a solar cell's relative spectral response [7]. In the laboratory, current–voltage tracing and spectral response are standard and complementary solar cell measurement techniques [8], so their recent incorporation in production line measurement allows lab analysis methods to be adapted to high-volume data in the production line for the purposes of pin-pointing areas of manufacturing improvements.

This paper explores the multivariate statistical information offered when both volume one-Sun *I–V* and spectral response data are available for large batches of passivated emitter, rear locally

Batch	Description
1	Baseline
2	Identical processing to batch 1, except for the type of furnace used for phosphorus diffusion
3	Identical processing to batch 1, except for the quartz tube used for phosphorus diffusion
4	Identical processing to batch 1, except for the tool used for rear passivation

Table 1. Description of the four solar cell batches.

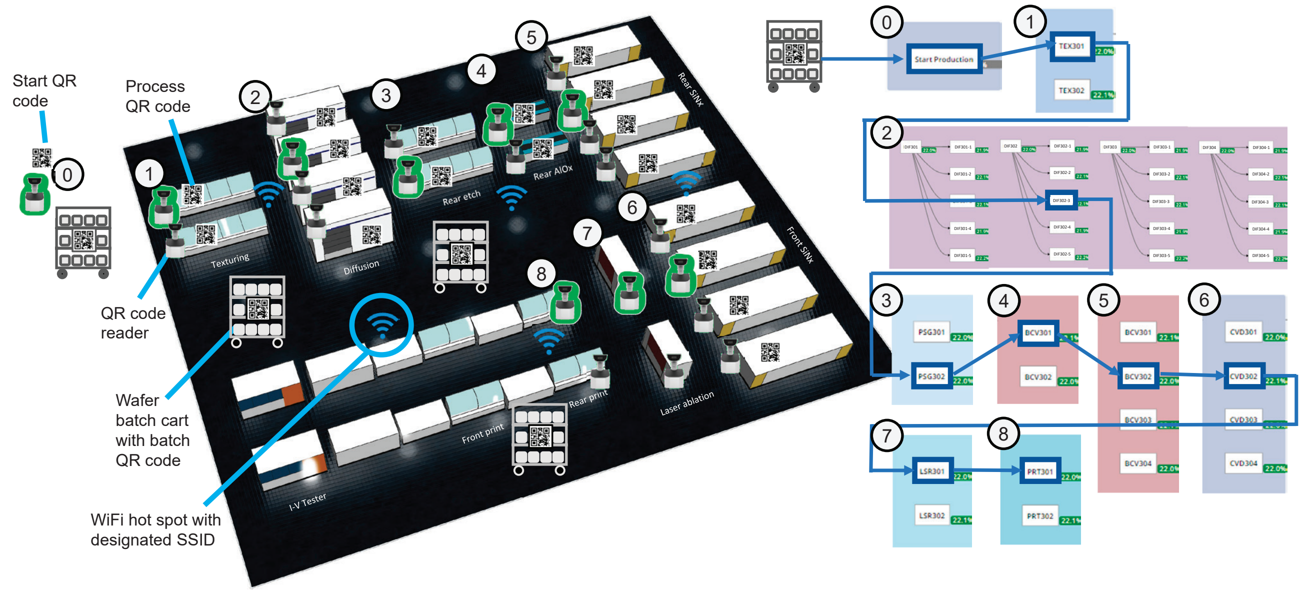

Figure 1. Batch path-tracking system using QR code pairing to record the check-in time and process tool/chamber at each step.

contacted (PERC) solar cells that have undergone different variations in manufacturing processes. For added value, two spectral response techniques are compared: 1) the traditional contacted method, which is based on short-circuit current measurement; and 2) a contactless quantum efficiency (QE) method, which is based on open-circuit luminescence emission measurement [9–10]. The two techniques are performed when the solar cell is exposed to monochromatic illumination. Both kinds of spectral response data are used in conjunction with one-Sun *I–V* data to perform intra-batch and inter-batch analysis.

Cell fabrication and tracking

Four batches of PERC solar cells were fabricated in a volume manufacturing environment. Each batch took a different route through the path of process tools/chambers to create four experimental splits. Table 1 summarizes the differences in the process paths taken by the four batches.

In order to verify that the batches did follow the intended paths, a batch path-tracking system using QR code scans was implemented to record the check-in times, and specific process tool/chambers used as the cassettes containing each batch were loaded for processing at each process step. The production facility operators were trained and instructed to perform the QR code scans using a handheld reader, which sent the batch QR code and process QR code scan pair to a server in real time. The server timestamped and logged these events in a path-tracking database. Other than logging the check-in events of the four batches, the server computer also consolidated the path data of all batches to give either a plant-wide view, or a tool-comparison view, in which the *I–V* parameters of batches moving through different tools could be compared.

The schematic of this path-tracking method is given in Fig. 1, which shows the mapping of the physical factory and tool space to the server database space, as presented on the manufacturing facility view screen. The corresponding process

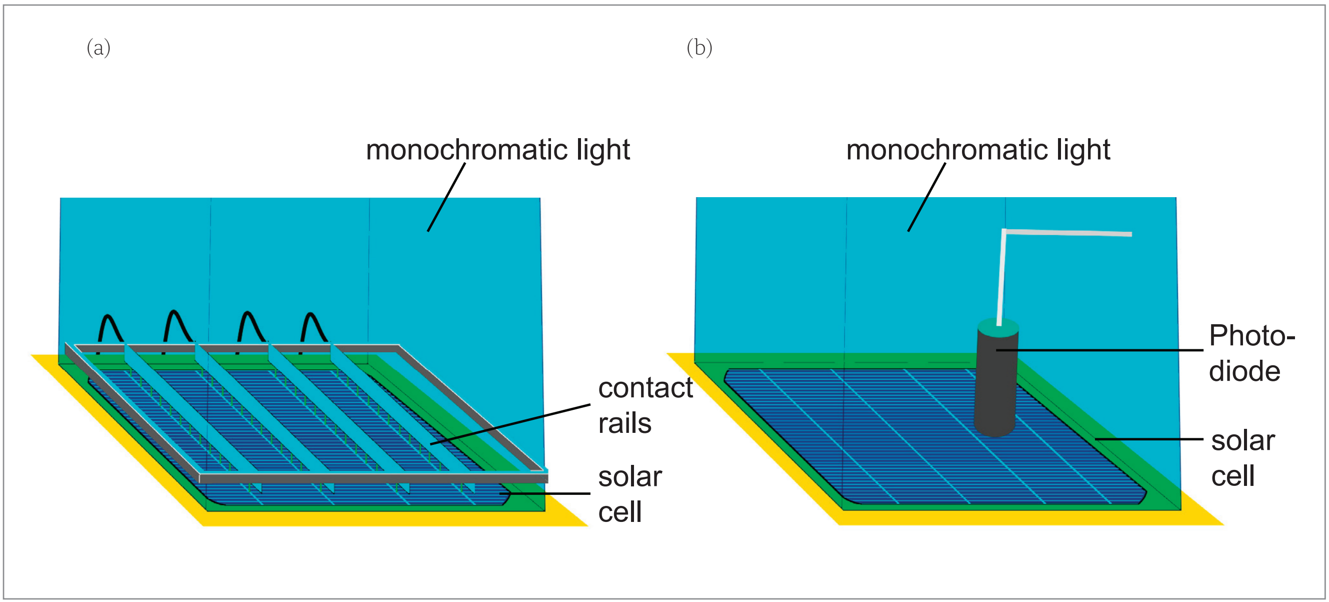

Figure 2. (a) Contacted spectral response measurement, with current being measured under short-circuit conditions. (b) Contactless spectral response measurement, with luminescence intensity being measured under open-circuit conditions. Both are performed using monochromatic illumination.

steps in the two spaces are numbered. For illustrative purposes, Fig. 1 also shows an example case where the path information of a batch is recorded. The highlighted QR code readers denote QR code scans, and in the plant-wide view screen, the blue boxes denote the recorded process tool/chambers that were used to process the batch.

I–V and spectral response measurement

All four batches of solar cells were metallized in the same print line and flashed by the same xenon-lamp-equipped *I–V* tester sorter. For each batch, about 500 contiguous cells were extracted for offline testing. The test sequence consisted of standard one-Sun *I–V* testing using an LED-based illumination, as well as the contacted and contactless implementations of spectral response measurements as described above and in Fig. 2. The contacted technique is based on short-circuit current measurement, and the contactless technique is based on open-circuit luminescence emission measurement. The contacted measurements are taken under monochromatic illumination at 395nm, 686nm, 799nm, 975nm and 1,060nm, while the contactless measurements are taken under monochromatic illumination at 390nm and 660nm.

Because the wavelengths of 686nm and 660nm are very near constant spectral response per unit cell active area, the measurements at these wavelengths can be used to normalize the measurements at other wavelengths. This procedure, while optional for the contacted measurement, is necessary for contactless measurement in order to generate meaningful results [10].

The normalized spectral response at 395nm or 390nm is called the *blue response*. It is highly sensitive to the anti-reflection coating thickness and refractive index, and slightly so to emitter passivation quality and emitter bulk recombination. For the contacted spectral response measurement, the response at 975nm or 1,060nm is called the *red response*. It is also highly sensitive to the anti-reflection coating thickness, and slightly sensitive to the base diffusion length.

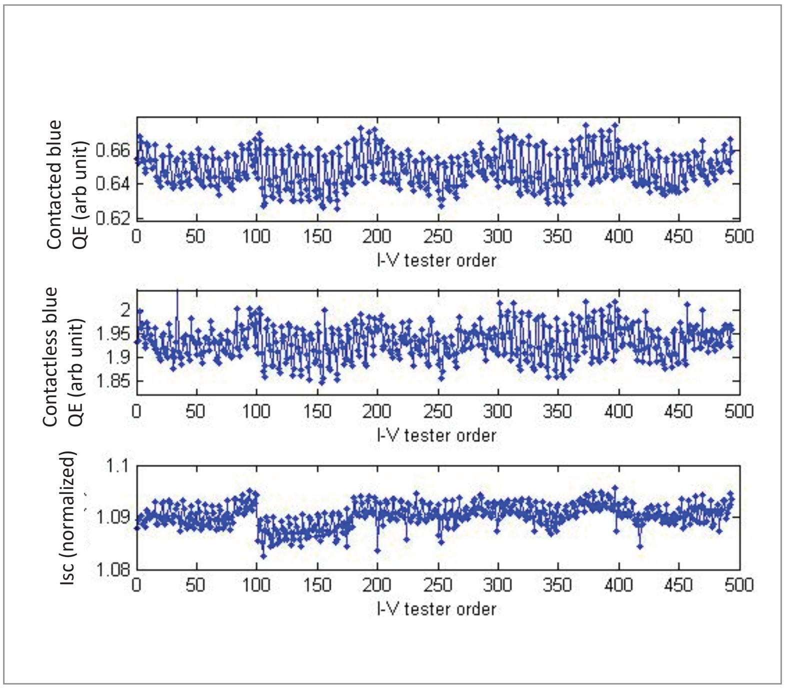

Figure 3. Blue response in contacted spectral response and contactless response, and the one-Sun short-circuit current (I_{sc}) for batch 4 measurement sequence.

Measurement results and discussion

Fig. 3 shows the blue response in contacted spectral measurement and contactless spectral

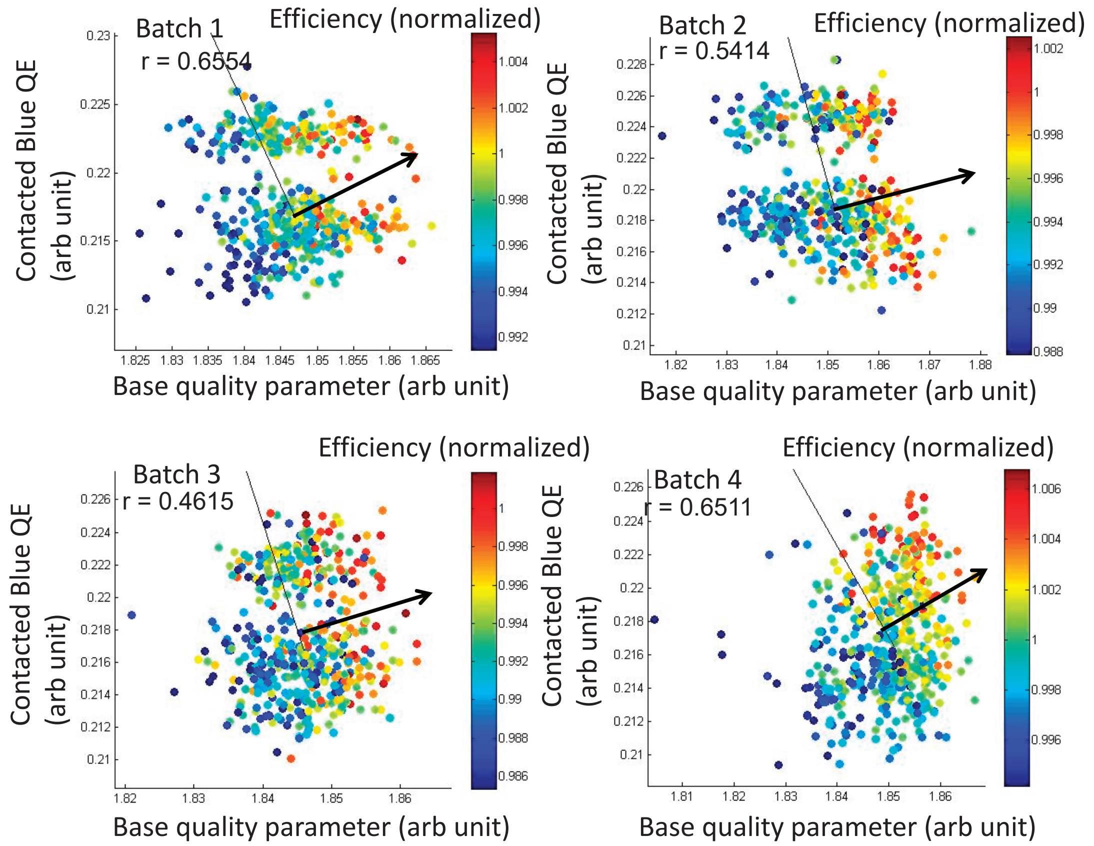

Figure 4. Intra-batch scatter plots of efficiency versus the contacted blue response and base quality parameter (derived from the IR response), each shown with the gradient direction.

measurement, and the one-Sun short-circuit current (I_{sc}) for batch 4, with the spatial cell ordering in the batch preserved. Clearly, in all three types of measurement, there is a periodic structure in the batch spatial sequence. In fact, this periodic structure is evident in all four cell batches, but for brevity only that of batch 4 is presented here. By using a correlation technique, it is found that the periodicity in the blue response is eight solar cells. Because this periodicity is observed only in I_{sc} in the blue spectral response, one can conclude that the periodicity is related to a process tool that influences the anti-reflection coating refractive index, which is most likely the silicon nitride (SiN_x) vacuum deposition tool.

Fig. 3 also shows that the contacted and contactless spectral response techniques produce similar results in the blue response. In fact, the correlation coefficients between the blue responses of the two techniques are r = 0.957, 0.832, 0.945 and 0.963, for the four batches, respectively, which is excellent. This shows that, in practice, the cells' blue response can be reliably obtained either by using the contacted spectral response method, preferably integrated in the I–V tester [8], or by using a contactless device situated at the end-of-line position, close to the I–V tester.

Having identified and briefly discussed this periodicity in the blue spectral response, it is now desirable to investigate how it and other spectral response results relate to cell efficiency. Fig. 4 shows, within each batch, the scatter plots of efficiency versus the contacted blue spectral response and a base quality parameter (which is derived from the red response), each shown with the gradient direction. As expected, in each case the efficiency trends positively with both the blue response and the base quality parameter.

Examination and use of the blue response can be a significant factor in improving finished cell efficiency and therefore production line yield. Observe from Fig. 4 that each batch has a bimodal distribution: a high blue response mode and a low blue response mode. The differences in median

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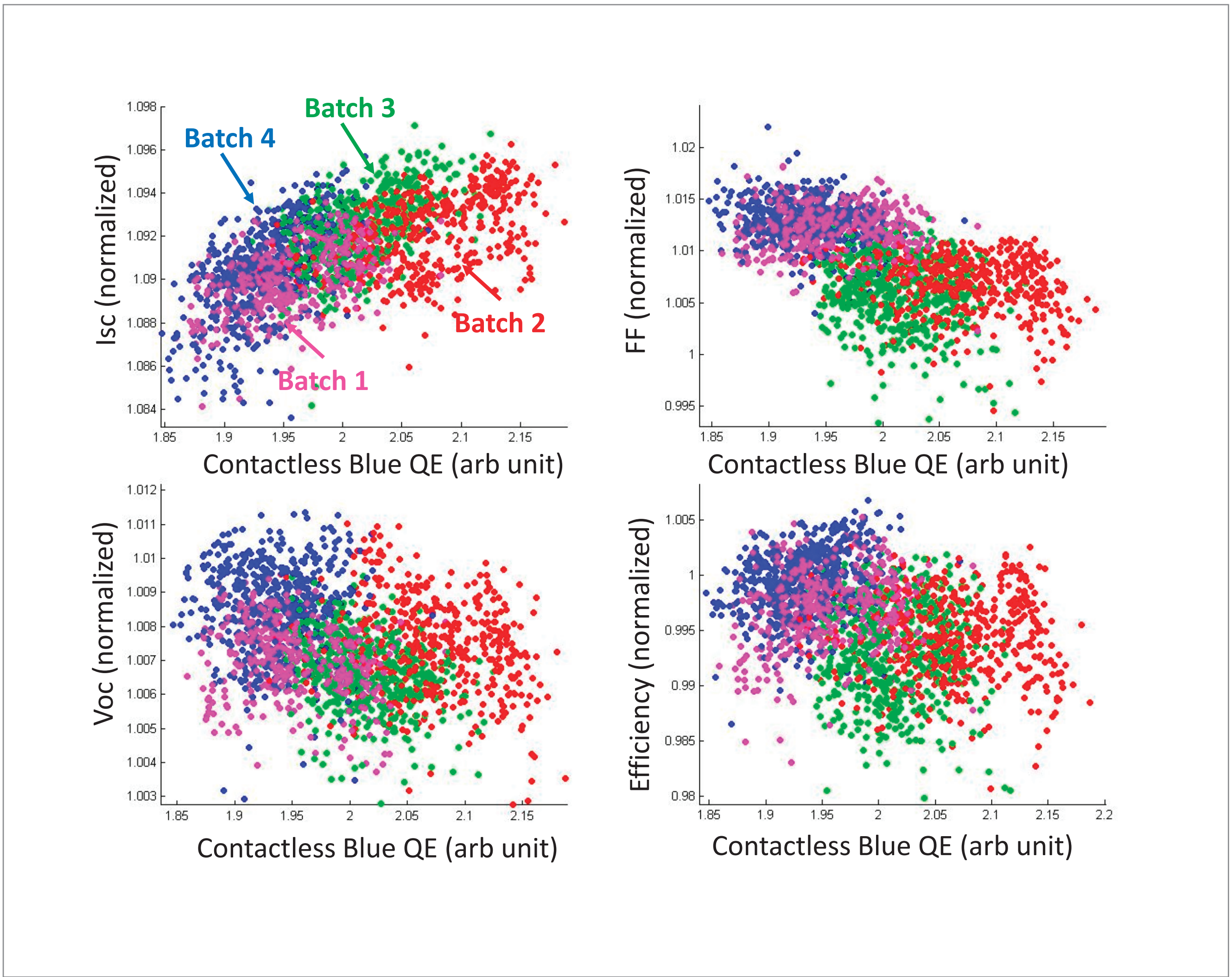

Figure 5. Inter-batch trends of contactless blue response versus short-circuit current (I_{sc}), fill factor (*FF*), open-circuit voltage (V_{oc}) and efficiency.

efficiencies between these two modes are 0.02%, 0.02%, 0.04%, 0.07% absolute efficiency points for batches 1 to 4 respectively. These differences are sufficiently significant to make it worthwhile to investigate, and, if possible, reduce or eliminate the SiN_x vacuum deposition tool inhomogeneity as a way to reduce the variance and possibly increase the mean of the finished cell efficiency distribution.

Additionally, it turns out that the base quality parameter explains an even more significant part of the total variance in efficiency. There is evidently an improvement in the base quality parameter for batch 4, which was subjected to a different rear-passivation recipe to that of batch 1. This improvement in base quality parameter largely explains the difference in the two batches' efficiencies. Thus, using the base quality parameter to interpret experimental splits – where the intended change is in the rear passivation – can lead to clearer conclusions, more accurate attribution of efficiency changes to the control variable, and potentially more efficient experiments that require fewer samples.

More inter-batch analysis can be carried out by plotting all four batches together in a set of two-variable plots. Fig. 5 shows four inter-batch trends of contactless blue response versus, respectively, short-circuit current (I_{sc}), fill factor (*FF*), open-circuit voltage (V_{oc}) and efficiency. Batches 1 and 4 (which differ only by their rear-passivation processing) have a nearly identical blue response and I_{sc}, while batches 2 and 3 (which were processed in a different type of diffusion furnace and in a different diffusion tube compared with batch 1, respectively) have distinctly different blue responses and slightly different short-circuit currents. Thus, the contactless blue response could be a parameter that is more sensitive to changes in emitter profile compared with *I–V* parameters, as evident in its ability to differentiate batches that have different emitter processing.

There is also a negative trend between the blue response and the fill factor among the batches. This trend makes sense if it is posited that emitters with higher surface concentration have higher Auger and surface recombination, and therefore lower blue response, while at the same time forming lower-resistance contacts with the screen-print metal lines, thus leading to a higher fill factor. A long-term inter-batch study of this trend

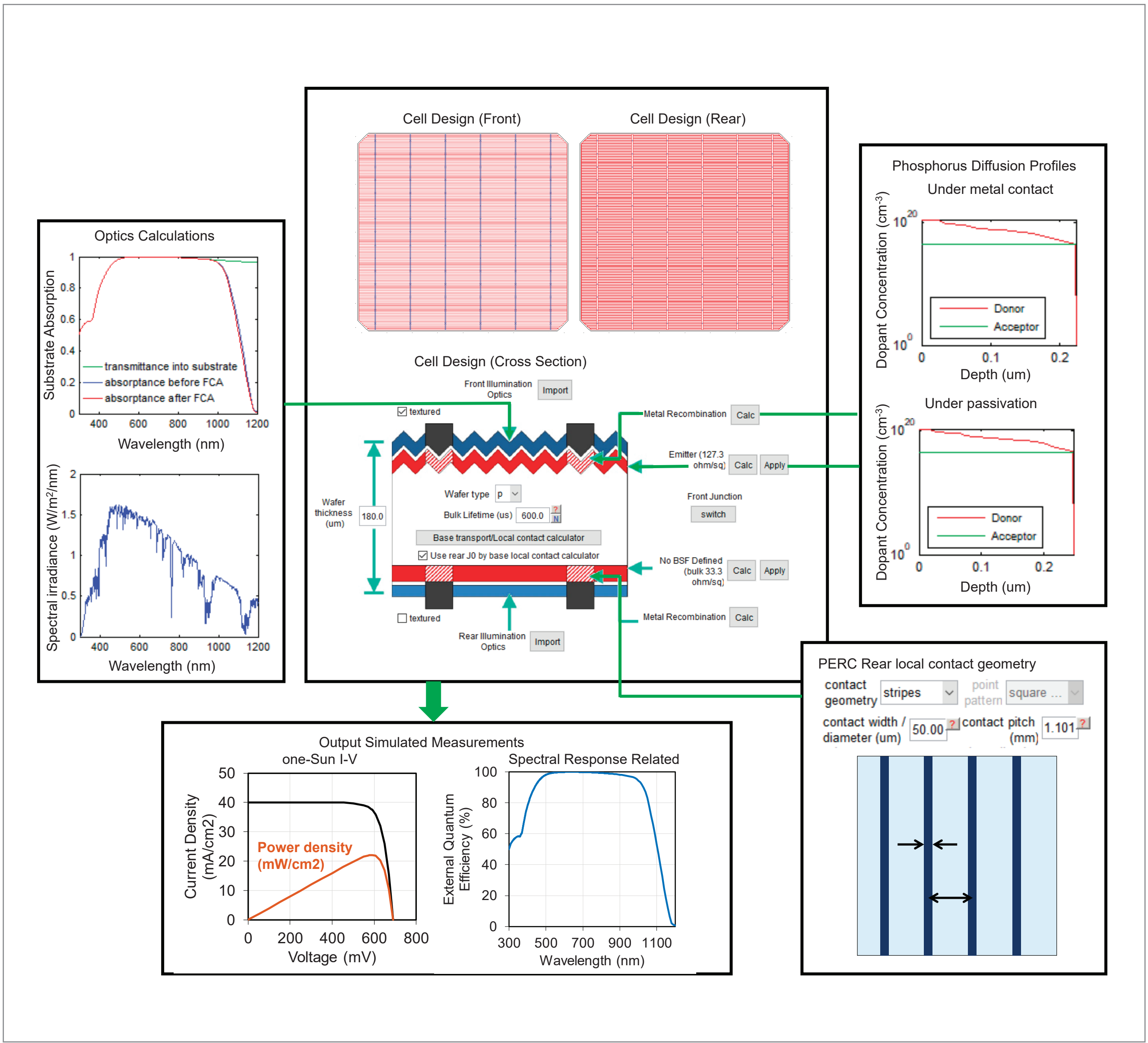

Figure 6. Physics-based device model for the PERC cell, which accepts as inputs various detailed cell parameters – such as emitter phosphorus diffusion profile, anti-reflection coating thickness and refractive index, and rear-passivation quality – and calculates both the one-Sun *I–V* and spectral response characteristics.

could aid emitter profile optimization by diffusion furnace process tuning.

Digital twin

As mentioned in the introduction, a digital twin for the solar cell manufacturing process can be considered to be akin to solar cell device models and fabrication process simulations. Indeed, in this work, as the starting point for the device model part of a digital twin, a detailed solar cell physics model created in Griddler was used, which is a finite-element model and simulation program for solar cells [11–12]. Griddler accepts as inputs various detailed cell parameters, such as emitter dopant profile, anti-reflection coating thickness and its refractive index, and rear-passivation quality (defined by the surface recombination velocity), and calculates both the one-Sun *I–V* and spectral response. As shown in Fig. 6, a physics-based device model was constructed in Griddler, using cell parameters typical of a PERC cell that would yield similar *I–V* parameters to those of the median solar cell in the production line batches described earlier.

While the Griddler model is useful for device design work – metallization pattern optimization, modelling the influence of material quality, evaluation of new diffusion recipes, and so on – it cannot interpret production line measurements in real time. Such real-time interpretation is necessary for continuous manufacturing-yield optimization and troubleshooting, unlike during device design. Indeed, as mentioned in Zimmer et al. [4], one of the most important points in modelling is to find the right balance between pragmatism and scientific rigour, as the latter may consume unnecessary computing power and render real-time processing infeasible.

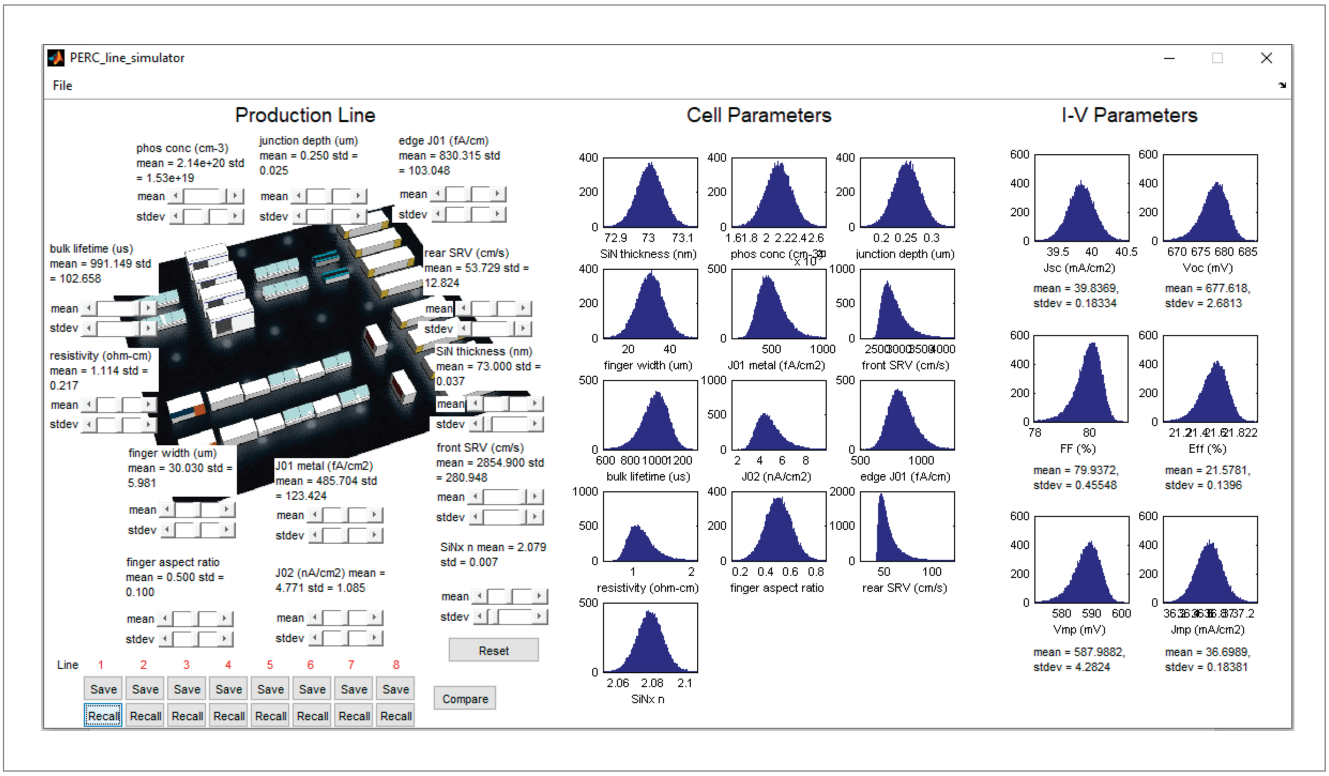

Figure 7. Yield-oriented model for variations in PERC cell fabrication. The model accepts as inputs the statistical distributions of the cell properties, and outputs the statistical distributions of the *I–V* and spectral response parameters (the latter is not shown in this figure).

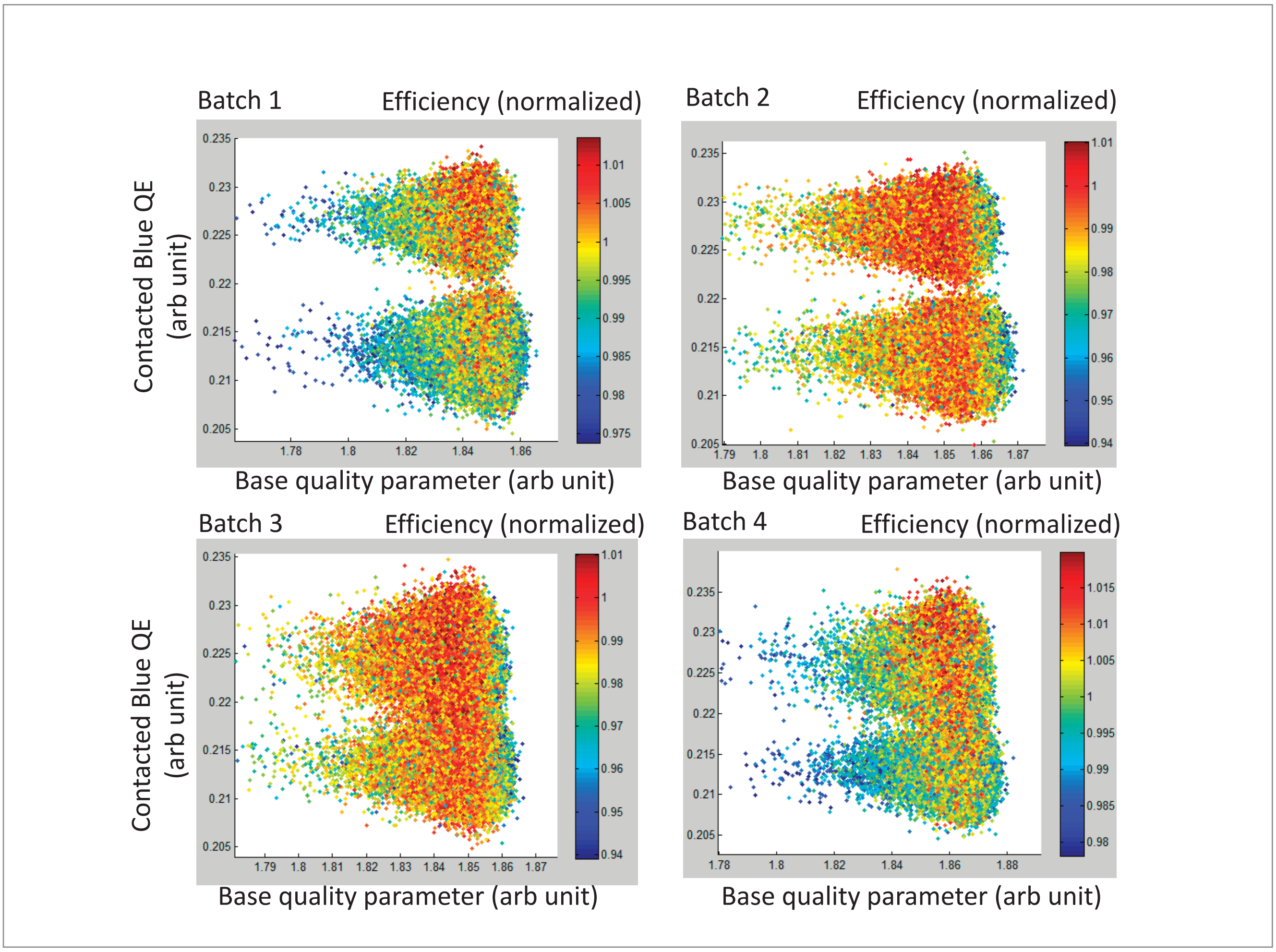

Figure 8. Interpretation of the spectral response data plots in Fig. 4, using the yield-oriented cell model, showing a bimodal distribution for each batch.

In order to render the Griddler device model suitable for employment as a digital twin, good use is made of the fact that the digital twin is intended for the interpretation of statistical distributions in which the underlying material properties and finished cell parameters are not drastically different from the median for most of the time. Therefore, the focus will be on a simple statistical model that yields the same results as the Griddler model when all input properties are at median values, and which performs well at predicting the rates of change in measurement values that are caused by variations in those properties that are relevant to manufacturing yield.

The resulting model for the PERC cell accepts as inputs the statistical distributions of the cell properties, and outputs the statistical distributions of the *I–V* and spectral response parameters, as shown in Fig. 7. This model is characterized as *yield oriented*, because it includes the variances (distributions) of input properties and shows the resulting finished cell parameter variances (distributions).

While it is a straightforward matter to model *I–V* and spectral response results on the basis of a given set of cell properties and their variations, the

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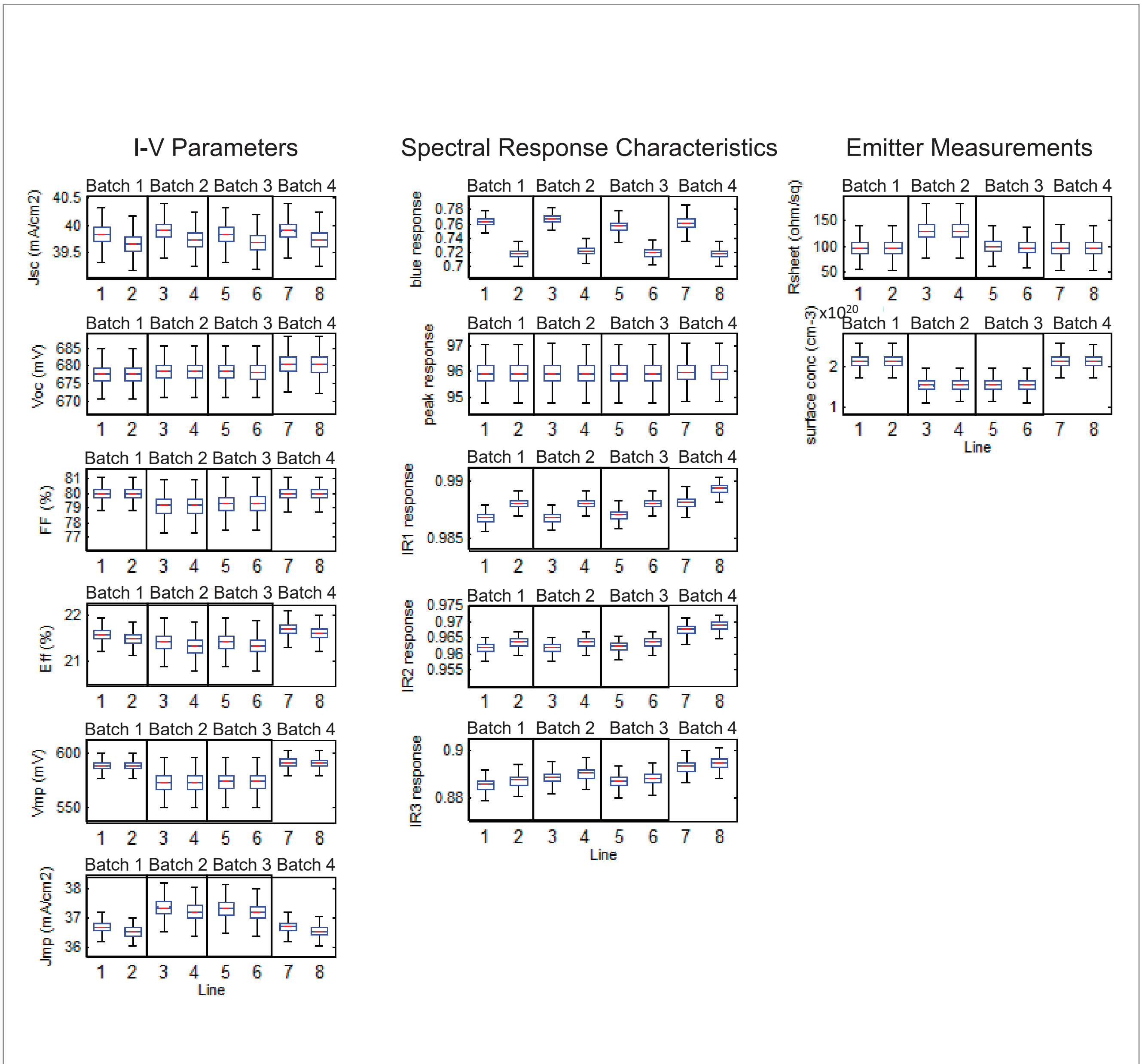

Figure 9. Box plots of the various modelled measurement characteristics for the four cell batches, using the yield-oriented model. In addition to *I–V* and spectral response parameters, the emitter sheet resistance and surface concentration are also modelled. The ability of the model to predict these latter properties offers increased depth of analysis and enhanced diffusion process control options for production lines that have inline doped layer measurement tools.

accuracy of the inverse approach – finding a set of cell properties that give rise to specific observed finished cell parameters – is prone to severe degradations by measurement noise, confounding factors and model inaccuracies. The model for deriving these properties must be designed to seek solutions within a plausible range of possibilities by setting certain rules, bounds and constraints, the details of which are beyond the scope of this paper. This allows a digital twin to be used to interpret *I–V* and spectral response data in a practical manner. As an example, referring to the spectral response data plots in Fig. 4, the model interprets the bimodal nature of the blue response in each batch as arising from corresponding bimodal variations in the anti-reflection coating refractive index. Fig. 8 shows the resulting plots of the spectral responses for the four batches.

Fig. 9 shows box plots of the various modelled *I–V* and spectral response parameters for the four cell batches, using the inverse yield-oriented model. Notice that each batch has two distributions of cell parameters, each with a different median for the anti-reflection coating refractive index, in order to reproduce the bimodal nature in the blue response. In addition to *I–V* and spectral response parameters, the emitter sheet resistance and surface concentration are also modelled. These latter modelled properties are to illustrate – for production lines equipped with inline emitter layer measurement capabilities [13] – that certain doped layer measurements be interpreted together with end-of-line cell parameters to form a more conclusive picture of the underlying causes of variations seen on the production floor.

Summary and outlook

This study of volume manufacturing data using four solar cell batches demonstrates the usefulness of inline spectral response measurements in the production line. First, by attributing patterns seen in the *I–V* parameters to the blue response or the base quality properties (derived from the red response), one can quickly identify the fabrication processes and their variations that give rise to these patterns, and also assess the impact of the process variations on finished cell efficiency. The spectral response data is often more sensitive than *I–V* parameters to variations in fabrication processes, thus potentially aiding pre-emptive maintenance actions or diagnosis of issues in the production line.

A suitably designed digital twin which combines the rigour of a physics model with the practicality of statistical models proves to be useful in performing real-time batch statistics interpretation. With a physics basis, the digital twin is sophisticated enough to consider a multitude of data, such as *I–V* and spectral response parameters, and possibly doped layer measurements in the future. With a statistical basis, it is built to handle high-volume, high-throughput data typically encountered in a solar cell factory. One can envisage the digital twin being used for yield-improving purposes, such as:

1. What-if analysis, e.g. predicting the benefits of employing engineering process control to reduce a certain process-induced cell property variance.

2. Root cause analysis to remedy and prevent out-of-control events.

3. An aide in experimental data interpretation in evolutionary operations to reduce the number of cells required in processing experimental batches.

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