Ramping Advanced Silicon Solar Cell Production with Virtual Wafer Tracking

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ABSTRACT

First Solar's TetraSun pilot production line featured single wafer tracking and sophisticated analytics. In this modern PV production environment, wafers are tracked virtually, with no physical (eg. laser) marking required, ensuring that no efficiency or yield loss is incurred, and no additional hardware is required. The tracking system provided the platform to develop techniques for (i) running experiments and line optimisation efficiently and with high statistical power and few unnecessary assumptions; (ii) ensuring quality control through the application of physics-based multivariate models to high dimensional data sets; and (iii) reducing the impact of yield loss events and accelerating root cause analysis. Such techniques were essential ingredients for the successful commissioning, ramp-up and operation of the novel, low-cost, high-efficiency TetraSun cell and module technology to 100 MW mass production.

INTRODUCTION

Modern solar cell manufacturing must evolve towards an enhanced emphasis on process control and quality. Photovoltaic manufacturing can be a relatively low margin enterprise, and so product and brand 'bankability' is a key prerequisite for business success and the mass deployment of photovoltaic modules. An enhanced focus on quality – that is the extent to which every cell can be made the same - will achieve this by improving production yields, lowering the risk of field failures, and improving the ability to continuously improve the production line. In the search for higher efficiency, the cell manufacturing process has a tendency towards complexity, meaning that an increasing number of factors can contribute to variance, and the embodied cost of such variance. It seems appropriate that the need to evolve is witnessed first in the higher efficiency 'premium product' segment, where quality (consistency of product) may be a key point of differentiation on which the manufacturer is able to build a market.

In addition to establishing a quality framework, other challenges are posed by the introduction of a novel high efficiency silicon solar technology into production at pilot scale. In order to unlock access to the high-return premium markets, a relatively higher cell efficiency must be achieved on a new toolset in the minimal possible time. The cost of a misinterpreted result, a lost lot, or an oversized experiment comprises not only the money spent on test repetition, but the opportunity cost of extended time-to-market or delayed revelation of the next optimisation opportunity.

To address these challenges, First Solar implemented a system capable of virtual individual wafer tracking, and harnessed that system (along with sound statistical principles, 'big data' approaches and a touch of engineering creativity) in its TetraSun silicon solar cell production line. Between late 2014 and mid 2016, the production line ramped up to an annualised run rate of 100 MW, achieving excellent efficiency yields (20.3% threshold) of > 99%, and median cell efficiency of ~21.1% [1]. The wafer tracking system was also central to the Engineering team's approach to experimental work, exemplified by the transfer and establishment of a new process to manufacture cells — with a median efficiency of ~21.9% and module power up to 330 W_p —to pilot scale [1].

The manufacturing execution system in the TetraSun production line features an individual wafer tracking system which records 1000s of data points for each cell produced. The system matches process conditions with the results of various metrology steps to reconcile a detailed history for the individual cell. The system provides all the benefits of laser marking and tracking [2- 5] without (i) potential efficiency loss; or (ii) a requirement for an additional write tool and several read tools. The virtual wafer tracking involves a central controller which records the movement of wafers as it is reported to that controller by the process and automation tools.

In this work, we discuss what we believe to be an industry-leading approach to leveraging such a wafer tracking system. We show, by way of examples, that the large volume of data collected by such a system was a key enabler to our efficient ramping up of production of our passivated contact cell technology. Our advanced approach to data collection and analysis allowed us to (i) spend minimal resources on conducting high resolution experiments and optimisations (such as wafer vendor qualification); (ii) rapidly identify and resolve yield issues; and (iii) apply new statistical approaches to ensure quality throughout the production ramp, even while fine-tuning process recipes towards their final state.

LEVERAGING IN-DEPTH UNDERSTANDING OF PRODUCTION VARIANCE TO DESIGN EFFICIENT EXPERIMENTS

It is usually difficult to conduct powerful experiments on a solar cell production line while also keeping the cost of those experiments under control. Powerful experiments, i.e those with a high statistical power, are those which have a high likelihood to resolve small differences in a magnitude-of-interest. Readers might be familiar with the statistical power afforded by fractional factorials, for example, which intentionally alias unlikely interactions with main effects, in order to reduce the burden of the experiment to fewer test conditions. Readers might be equally familiar with the concept of sample independence. Most solar cell production lines are afflicted by an unfortunate combination of (i) autocorrelation and sample interdependency and (ii) the need to track an experiment through a production line involving paper lot-sheet tracking. Autocorrelation occurs when the performance of a cell is more likely to be similar to the cells made at the same time, than it is to be similar to any given cell taken at random from production. This means every sample cannot be considered to be independent and this affects statistical decision making. Meanwhile, paper lot-sheet tracking is prone to human error and necessitates large batches. Under manual tracking, the most difficult aspect of experimental design might be negotiation with an operations team who inevitably seeks to minimise the time lost to run a special condition (so wishes, for example, not to run ‘repeats’ of experimental splits).

While sample interdependency remains present in the TetraSun line, the incorporation of individual wafer tracking allowed us to develop an algorithm to take the autocorrelation phenomenon into account, then appropriately size experiments and tune analysis. The algorithm slightly modifies the standard calculation of experimental power, affording high likelihood of detecting a particular experimental effect, while decreasing the vulnerability of the experiments to incorrect conclusions that might be brought about by autocorrelation, batch effects and so on. Lot size was hence reduced, no manual tracking was required, more splits could be tested, and experiments were both cheaper and more powerful. Often, additional randomisation strategies were applied in order to enhance experiment resolution. The closed loop of continual improvement became faster and more sensitive to small changes.

Autocorrelation results in incorrect conclusions (false effects or Type I errors) in experiments

A typical set of solar cell open circuit voltages is described in the time series of Figure 1. The analysis in the centre of that Figure reveals that the data has an in-built A-B-A-B trend; this probably derives from the fact that at the first automation station in the production line, stacks of wafers are loaded simultaneously into the subsequent tool from two magazines. As a result, the natural trend is for the production line to receive wafers from source A, then B, then A, then B and so on. The autocorrelation lags demonstrate that the wafer source has an impact on the final cell open circuit voltage. Of further interest is the observation of the right hand side of Figure 1, which plots the mean of each group of 5000 consecutive wafers tested. These mean values vary by much more than would be expected if the individual cells were independent. This is just another way of demonstrating the impact of autocorrelation. If an experiment happened to be run at this time, it is possible for this variance in the mean of these groups to be interpreted as being the result of the experiment, if it is not correctly analysed with respect to the sample independence.

This kind of potential misinterpretation can be expensive. Though misinterpretation can be avoided by appropriate retrospective checking of the statistical assumption of sample independence, it is best to design experiments that are relatively insensitive to such effects.

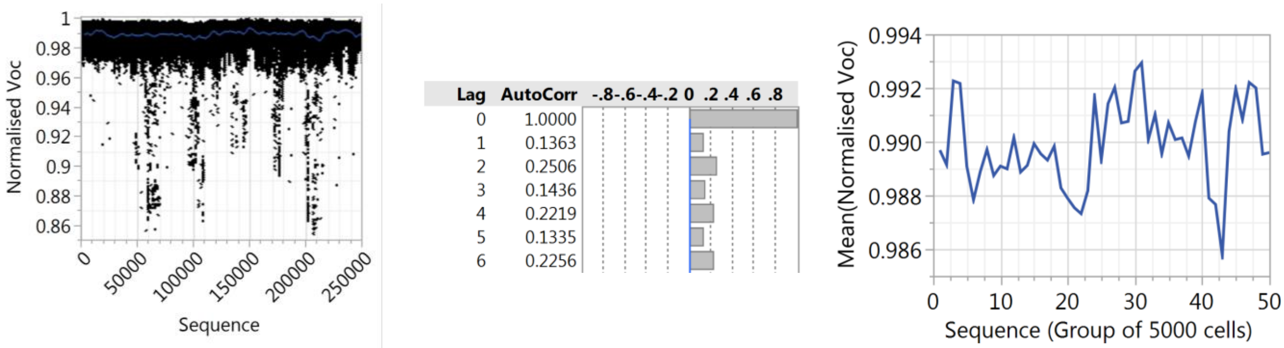

Figure 1: An exemplary time series of 250k solar cell open circuit voltages. At right, every cell is plotted in order of final test. Centre, the results of an autocorrelation appears to reveal that odd and even cells are correlated to one another more than to the remainder of the cells in the population. At right, the same data is aggregated into groups of 5000, as might be the case for a typical experiment featuring a comparison of treatments with large batch quantities.

Optimal Sizing of an Experiment

In PV production lines, when people are aware of the potential for making incorrect conclusions in relation to assumptions about sample independence, the typical approach is to conduct an experiment in lots of typically anywhere from 100 to 1000 cells, and for the statistical analysis to be done on the average value of the “lot”. The main problem with this approach is a huge loss of statistical power, without knowing whether the averaging is done with the most optimal number of samples. The optimal number would be where the averaging is as small as it needs to be for the average values to be independent for the purpose of the experiment analysis. If a set number of samples is chosen for a “lot”, sometimes this may be more than necessary for a given experiment and sometimes it may be insufficient to eliminate the dependency issue. The motivation of an experimental sizing algorithm is to be able to actively set optimal conditions for experimental analysis. This then motivates the ongoing improvement of the line for the purposes of conducting experiments, such as by identifying and ameliorating the causes of autocorrelation through techniques such as sample randomisation.

Description of the algorithm

The algorithm features a retrospective analysis of baseline production data, with a specific focus on the impact of autocorrelation and batch effects. The general approach is to “imprint” different theoretical experimental conditions onto the baseline data and see which ones would have generated “false positives” A false positive would be found when in any simulated experiment, we conclude to *reject* the null hypothesis. We know this to be a false positive because the data is only baseline data containing no intentional splits, representative of the normal situations where experiments are conducted. The algorithm generates, for a given experimental condition, a value less than one which is taken to be a “degrees of freedom multiplier” which would be necessary in that baseline data set and that experimental condition to have the false positive rate at 5% (a typical level for a false positive rate or type I error). In the experimental analysis, the actual number of samples is multiplied by the degrees of freedom multiplier to give the value for the number of independent samples in the experiment. This degrees of freedom multiplier was also used to calculate the statistical power of the given experimental design. Choices are then made about experimental design which optimise statistical power for a given size of resource (raw materials and operational resources) required for the experiment.
The specific calculations in the algorithm are –

- A set of baseline data is obtained, as large as possible, with data ordered by the run order at a specific tool of interest
- A theoretical experiment is “run” in the data by
    - Forming the data into a particular number of repeated groups of a particular size representing a theoretical experiment.

  - Calculating the sum of squares (SS_{model}) for these groups and a sum of squares (SS_{error}) for the error, and an F ratio using the degrees of freedom and assuming every sample is independent.
  - The probability is calculated, using the chi-sq distribution, that this value of the F-ratio occurs through random chance. In autocorrelated data, these probabilities would always be well below 5% due to the error in assuming every sample is independent.
  - The same grouping is repeated many times through a large baseline data set, giving a large set of SS_{model} and SS_{error} values that can be used to calculate a large set of F-ratio values and probabilities.
  - A degree of freedom multiplier (<1) is calculated so that probability derived from the F-ratio value is only below 5% on 5% of the occasions of the theoretical experiment being conducted within the data set.
  - Future experiments conducted in similar baseline conditions use this degrees of freedom multiplier in calculation of statistical power, and in the statistical analysis.
- This is repeated for different theoretical experiments of different group sizes and different repeats.
- The analysis is also conducted separately for all of the different performance parameters that are statistically assessed in an experiment, and for different sample orderings at different tools.
- This entire approach is run as a software script weekly on baseline data to automatically generate the information with which to optimise the design of experiments.

While this is a fairly detailed process, there would be several analogous approaches to this that achieve similar ends. The degrees of freedom multiplier approach was used because it is a convenient input to be used together with the commercial JMP statistical software, marketed by SAS. JMP is used at First Solar as a standard tool for statistical analysis. An equivalent approach could also be used to generate an ideal grouping size for averaging data, although in many lines this is frequently an operational convenience as much as a statistical analysis tool. There is not always the same flexibility to continually change this number to any value without the aid of the sophisticated wafer tracking. Nonetheless, any line would benefit from this analysis to make sure the experimental approach is close to optimal and the error rates are under control. The degrees of freedom multiplier approach and the group average approach will also produce different outcomes in situations where the data sets are strongly non-normal, and averaging is needed to obtain a more normal distribution (thanks to the central limit theorem). This was not an area of strong concern in the TetraSun production line.

<u>Example of algorithm output</u>

The algorithm was applied to the data of Figure 1. The result is plotted in Figure 2. The color represents the size of the experimental effect which would be resolvable with a 95% probability, if it existed. The size of the effect is expressed generically in terms of the proportion of a stand deviation in V_{oc} as it typically done. Note that the real-world data used here does not result in smooth contours. The complex interactions occurring in the production line preclude predictability except at the macro-scale (the nature of batch sizes, buffers, operations rules and so on make the production line situation complex). In general, larger group sizes and more repeats resolve smaller differences between two populations. Comparing the colored contours to the overlay, note that repetition of settings is an extremely powerful way to reduce experimental cost (the overlay signifies the total number of samples required for the experiment). The engineer might use this result to design an experiment to resolve a difference between two settings of 0.4σ; she could choose to run 8 repeats of 200 samples (1600 total wafers per condition), or 4 repeats of 5000 samples (20000 total wafers per condition). The engineer would surely do everything in her power to select the former, though it is sometimes the case that settings are 'hard to change' (eg. a furnace temperature change may require a long period of stabilisation), so opportunity cost must be weighed against sample cost. With automated wafer tracking, this experimental design is at least limited by the nature of the equipment and the process, as opposed to the ability to paper track lots through a production facility.

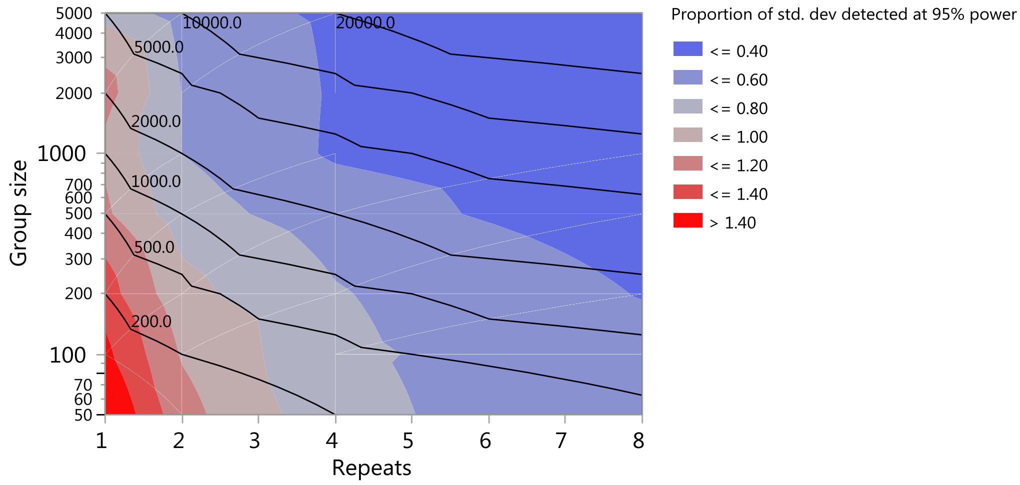

Figure 2: Shown in color fill is the calculated experimental capability (size of the effect resolvable at 95% power in terms of the standard deviation of the baseline data) as a function of the group size and the number of repeats. The black line contours denotes the total number of samples required (ie. the cost of the hypothetical experiment). This describes an experiment comparing two levels, but it can be repeated for multiple levels or regression experiments

An example of batch experimentation using virtual wafer tracking

Virtual wafer tracking helps unlock continuous improvements in performance such as is shown in Figure 2, where a large number of repeats of small batches are used to resolve very small differences (to perform very fine optimisations). Without virtual wafer tracking, it would be necessary to follow numerous sample groups through the production line using a paper or human system – in our estimation the associated overhead would eliminate the cost advantage of using fewer wafers in the experiment.

In this example, we set a batch process to automatically switch recipes for every batch load of wafers in the equipment, through a set of 25 pre-defined recipes. Figure 3 shows the result which indicates that the optimum performance is achieved with a high value of Factor A and a low value of Factor B. This experiment tested only 400 wafers per level and required no intervention other than to set the recipes on the equipment. The reader can imagine the extension of such an approach to evolutionary operation [7], where very small differences are detected with very large ‘experiments’.

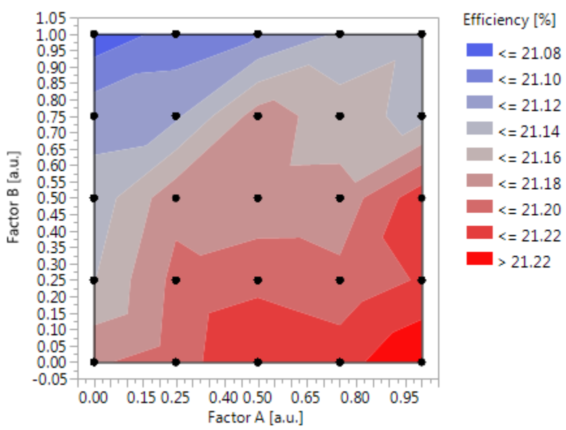

Figure 3: Contour plot of final cell efficiency shown as a function of two process parameters related to one of our process steps.

The benefit of virtual wafer tracking – extreme example of wafer vendor qualification

Silicon wafer vendor qualification is a task made incredibly simple by virtual wafer tracking. Suppose we set a technical limit that the new vendor must perform at a certain yield or within a certain limit (eg. in V_{oc}) of a known-good reference. One option would be to run two large batches; one from the known-good vendor, and one from the control. A better option is to run an experiment in which the two wafer vendors are loaded into the production line alternately then compared pairwise (in this case one would seek to determine whether the mean or distribution of the pairwise comparisons was acceptable). In the TetraSun production line, the first process tool loads from two magazines alternately. It was relatively simple to set magazine A to load the known-good vendor and to set magazine B to load the new vendor. The virtual wafer tracking system then delivers a set of performance data together with the vendor name and loading time. It is relatively simple to transform this data set into a set of pairs of wafers loaded and processed side-by-side. The test statistic can be the difference between each pair, and this test statistic has virtually no autocorrelation. Every pair is therefore considered a truly independent sample. As a result, very high statistical power is achieved and the experiment becomes a very sensitive assessment of differences in material quality between vendors.

LEVERAGING MULTIVARIATE MONITORING TECHNIQUES TO IMPROVE PRODUCT QUALITY

Manufacturing quality is a measure of the ability to make the same thing every time. High quality requires a focus on, and understanding of, the sources of variance in production. With individual wafer tracking, it is possible to employ more advanced multivariate analytical techniques to identify process deviations or quality problems that are not identifiable by examination of the variance of individual parameters [6]. Moreover, it is far simpler to correlate and eventually attribute these excursions to process and equipment issues, as is shown in the example below.

An advanced multivariate technique for monitoring the contributions to cell series resistance was applied during the ramp phase of the TetraSun production line. The technique leverages individual wafer tracking, combining mid sequence metrology (resistance of various doped layers) and end-of-line metrology (grid resistances on front and rear as well as an extracted lumped series resistance for the cell). For a typical and well-behaved group of cells, the final cell series resistance is predicted by a model combining the aforementioned components and arrives at a prediction with a reasonable fit quality (R^2 usually between 0.5 and 0.9). This is demonstrated by plotting the control chart (see Figure 4 (a)) of R^2 for fits to consecutive groups of 5000 cells produced. Although R^2 does not appear to be a particularly stable parameter across all ~800k cells represented in this timeframe, one can readily distinguish the 'crash' in R^2 into an out-of-control state from groups ~150 onwards. Whilst in periods of 'normal behavior' the typical relationship between modelled and actual series resistance is similar to the one illustrated in Figure 4 (b), in the period beyond group ~150, the relationship devolves to the one illustrated in Figure 4 (c).

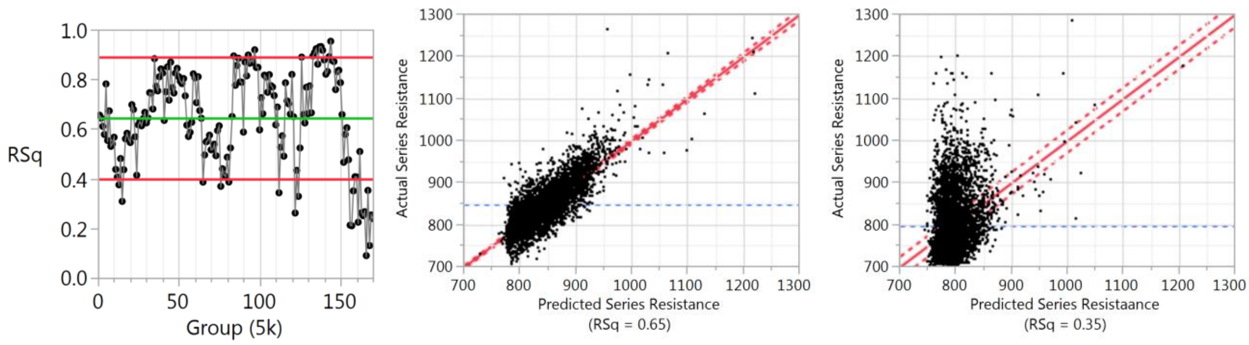

Figure 4: (a, left) A control chart for the quality of the fit of the series resistance model, with an excursion to low R2 in the groups > 150. (b, centre) The typical behavior of an in-control process; where the predicted and actual series resistances are highly correlated (group = 1). (c, right) Atypical, out-of-control behavior, with the tail of actual series resistance poorly described by the prediction (group = 158).

During the aforementioned out-of-control period, the predictive power of the variance model dropped considerably, but with minimal change in the variance of the series resistance itself. samples from the high tail (above the best fit line in Figure 4 (c)) are described as having an "un-parameterised" series resistance. In this case, the cells had unusually high contact resistance. They were immediately identified, with further characterisation (leveraging the individual wafer tracking history) identifying the root cause at a process well upstream of the final test. Subsequent tests revealed that such cells had poorer performance in accelerated degradation (reliability) testing. In this case, the focus on variance, using variance models, facilitates a high level of real time and predictive quality control. If these cells were not identified by the variance model, they would have otherwise been unremarkable in their performance and they would have been fielded in modules, with a higher-than-usual likelihood of becoming a future warranty liability.

REDUCING TIME-TO-REPAIR OF YIELD LOSSES

To achieve high yields in a mass production line it is necessary to track down ever less frequent problems and solve them. As the occurrence of a defect becomes less frequent, traditional methods to find the root-cause of the problem become more difficult to apply.

The TetraSun production line measures every cell for hotspot severity in order to avoid dangerously high temperatures in modules in the field. A number of different kinds of defects can cause a hotspot failure and lead to yield loss. Figure 5 (a) shows the hotspot severity for all cells processed in a particular slot inside one production process. It's clear from this data that slot 7 has significantly worse performance than all other slots. Further investigation of the location of the hotspots on the wafer shows that the failures in slot 7 were all in the same physical location (see Figure 5 (b)), unlike other failures which appear randomly distributed. This insight led directly to the root-cause of the problem (scratches caused by machine automation).

We were able to very rapidly detect, analyse, and solve a problem which was giving a 0.7% yield loss in a matter of a few hours owing to the very detailed set of data we collect on every individual wafer as they progress through the production line. Without this individual tracking it would have taken weeks to track down a problem of this magnitude.

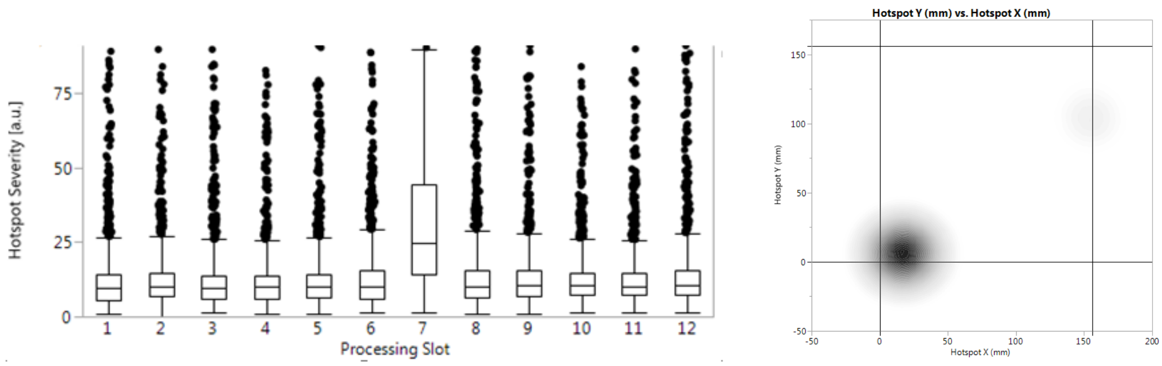

Figure 5: (a, left) Hotspot severity shown for the processing slot for one process. (b, right) Hotspot location heat-map for slot 7 as a function of the physical position on the wafer (156mm wafer edges shown as a guide).

CONCLUSIONS

Individual wafer tracking has been invaluable for the ramp up, diagnosis and optimisation of the TetraSun pilot production line. In order to extract the full benefit of wafer tracking, several novel and leading-edge approaches to data analysis were adopted. Algorithms were developed to optimise the use of experimental resources and substantially shorten the cycle of continuous improvement. Advanced mutlivariate statistical analyses were used to monitor and identify reliability issues in real time. Although some expertise and small investment in time is necessary to conceive of and tune all of these analysis techniques, once set up they can actually run in a largely automated way and provide for a sophisticate data analysis without requiring ongoing time and attention from company specialists, as would typically be the case for more in depth analysis. Used together, these approaches drove the rapid development and demonstration of a novel, high-efficiency cell process in mass production while also maintaining extremely high standards of quality.

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