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A combined Statistical and TCAD Model as a method for understanding and reducing variations in multicrystalline Si solar cell production

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Abstract

Monitoring the I-V parameters in mass production yields a distribution that cannot be understood in a simple manner. For example, if V_{oc} varies greatly, it is not obvious whether this is mainly due to variations in the bulk lifetime or in the surface passivation or due to other sources.

In this work, we develop a method where statistics is combined with numerical device modeling to obtain a physical interpretation of the observed variations. In the first part, we derive a multivariate statistical model to extract the main influences of fabrication fluctuations on the I-V parameters. This statistical model is based on cell parameters measured on a representative sample of solar cells from production. In the second part, we develop a computer-aided design (TCAD) device simulation model for multicrystalline Si solar cells. This TCAD model quantifies the I-V variations on a physically sound basis. However, the number of simulations is grossly reduced by feeding in solely the main influences obtained from the statistical model. In the third part, we verify this method by comparing the calculated distribution with production data.

This model is used for optimization strategies for higher cell efficiency, smaller variations in cell parameters and improved yield in mass production. Furthermore, we will apply our methodology to advanced cell concepts. It will allow the early consideration of production fluctuation in device simulation of advanced cell concepts, and therefore a realistic assessment of such concepts.

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Keywords: multicrystalline silicon solar cells ; device simulation

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1. Introduction

The goal to understand and reduce variations in semiconductor processes is an important task for mass production and Design for Manufacturing (DFM). Methods based on statistical models and physics-based simulations were developed for MESFETS [1] and bipolar transistors [2], which use different strategies to predict variances. The method proposed here combines the evaluation of measured parameter distributions and device characteristics in production. This method enables us to use I-V monitoring as a specific feedback for production improvements.

2. Statistical Model

The aim of a statistical model for production monitoring is to understand how the distribution of efficiency depends on the various measured variables and their distributions. In this paper, we perform a statistical analysis to identify the major influences on cell efficiency. To keep the measurement effort practical, we keep the sample size to 350 cells. For this statistical analysis [3] we consider all available optical and electrical parameters. In particular the parallel and series resistances, the deviations from the ideal IV curve (J_{02}), the quantum efficiency at different wavelengths, emitter and base doping, the characteristics of the reflectance curve and metallization properties such as area and contact resistance. We test the significance of every parameter as a predictor for cell efficiency by means of a multivariate regression analysis, applying a rather strict significance level of less than 0.01 as the criterion for inclusion. We prove the normal probability assumption for the residuals, and this ensures that the model is consistent. Finally the model with the highest coefficient of determination (adjusted R-squared) is chosen. Based on this model, a Pareto analysis shows that there are the following three main influences on the efficiency distribution:

1. the bulk diffusion length, obtained from quantum efficiency monitoring using the Basore fit [4], which is mainly related to the bulk lifetime τ_{bulk} ;
2. the reflectance at the minimum of the reflectance curve as a measure for the total shading due to the metallization, and
3. the lumped series resistance derived by the double light method using a HALM IV-tester [5].

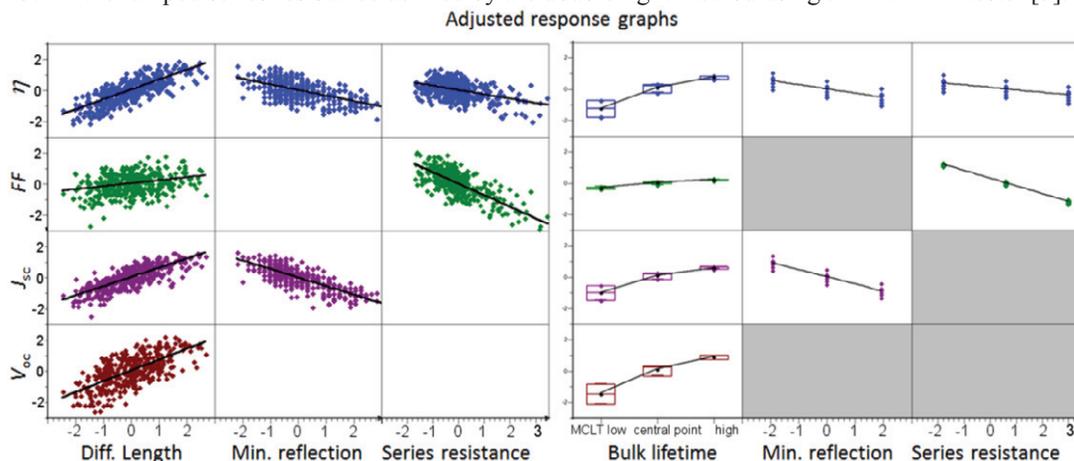


Fig. 1. (a) Multivariate statistical regression model for the mc-Si cell parameters, based on measurements; (b) Multivariate statistical model for the mc-Si cell parameters calculated with the TCAD simulations; both with a significance level less than 0.01 as the criterion for inclusion. All values are studentized i.e. taking ((value – calculated mean) / calculated standard deviation)

Based on these results a simplified multivariate statistical model, containing only the three major influences is used as the case study for our analysis. Fig. 1(a) shows the multivariate statistical model for cell efficiency η , fill factor FF, short-circuit current density J_{sc} and open-circuit voltage V_{oc} . It is an “adjusted response graph” where all values are “studentized” i.e. taking (value – calculated mean) / calculated standard deviation [3]. Apparently, V_{oc} depends in this model solely on the bulk diffusion length (the other parameters are insignificant). The short-circuit current density J_{sc} depends on both the bulk diffusion length and the reflectance at the minimum of the reflectance curve, which is a measure for the total shading due to the metallization. The fill factor FF depends on the lumped series resistance and slightly on the bulk diffusion length (via FF_0). Consequently the cell efficiency depends on all three major influences.

3. Technology Computer-Aided Design (TCAD) Device Simulation

The principal approach is to simulate an entire multicrystalline silicon solar cell as a parallel connection of 2-dimensional instances as indicated in Fig. 2 (a). The input parameters are obtained from a small sample of solar cells that was very well characterized off-line. For example, the bulk lifetime distribution of each cell is obtained by etching away the emitter and the BSF and by passivating the new surfaces with Al_2O_3 . Each image of $\tau_{bulk}(x,y)$ was then discretized in a lifetime histogram having a number n of lifetime values $\tau_{sim,i}$ with corresponding areas A_i , where the sum of all A_i is the total cell area. We then simulate a sequence of n monocrystalline Si cells, having the homogeneous lifetime $\tau_{sim,i}$, and obtain their I-V curves. To obtain the I-V curve of the mc-Si cell, we feed the simulated I-V curves into a numerical spice circuit model, using A_i as area factors. The circuit approximates the lateral current flow within both the semiconductor material and the metallization.

We use Sentaurus Device from Synopsys [6] to solve the complete set of semiconductor equations. The physical models of Refs. [7] and [8] are applied. All dopant profiles were independently measured with the electrochemical capacitance-voltage technique (ECV), and the front surface recombination velocity was adjusted such that the saturation current-density J_{0e} of the emitter, measured with the procedure of Kan and Swanson, is reproduced on independently fabricated samples.

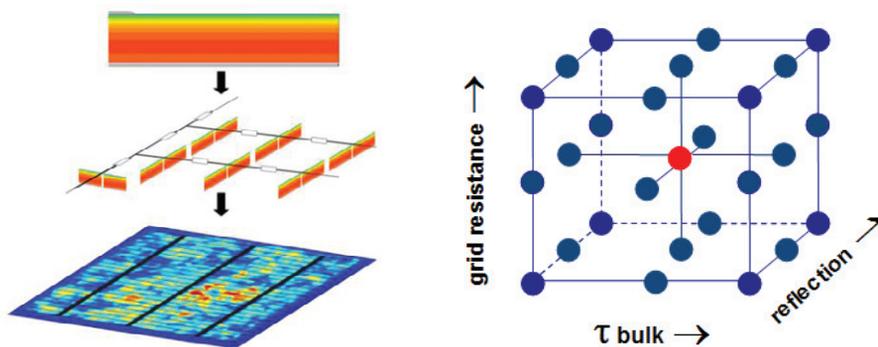


Fig. 2. (a) Simulation approach for a mc-Si cell: a 2D TCAD model (top) is combined with a circuit (SPICE) simulation (middle) to represent the entire solar cell (bottom); (b) Design of Experiment (DoE) for feeding variations into the TCAD model

4. Combined Statistical and TCAD Model

To incorporate the influence of process variations into the TCAD model, the three parameters identified in Chap. 2 (having a major impact) were varied in a systematic, full-factorial Design of Experiments (DoE) as shown in Fig. 2 (b). As central point the median (50%-percentile, P50) value was chosen (taken from the statistical model). The variation in this study was done within the interdecile range (P10-P90), in order to include the entire variation but without clear outliers.

It should be pointed out that in multicrystalline cells, τ_{bulk} is not a single value, but a distribution. Therefore, applied the TCAD model to various within-the-wafer distributions: two wafers for the P10 (low lifetime), three for P50 (average material), and two for P90 (high lifetime) to fit the above discussed P10-P50-P90 criteria.

The results of these TCAD simulations are evaluated in Fig. 1 (b). As a major outcome of this paper, the principal dependencies are well reproduced by the statistical model based on the TCAD simulations. Additionally, Fig. 3 even demonstrates that the distributions of cell efficiency are well reproduced. Please note that the upper and the lower bounds are correct. The slight overestimation of the efficiency at the main distribution is due to the neglecting of additional variations (e.g. emitter and BSF) and will be improved in extended models.

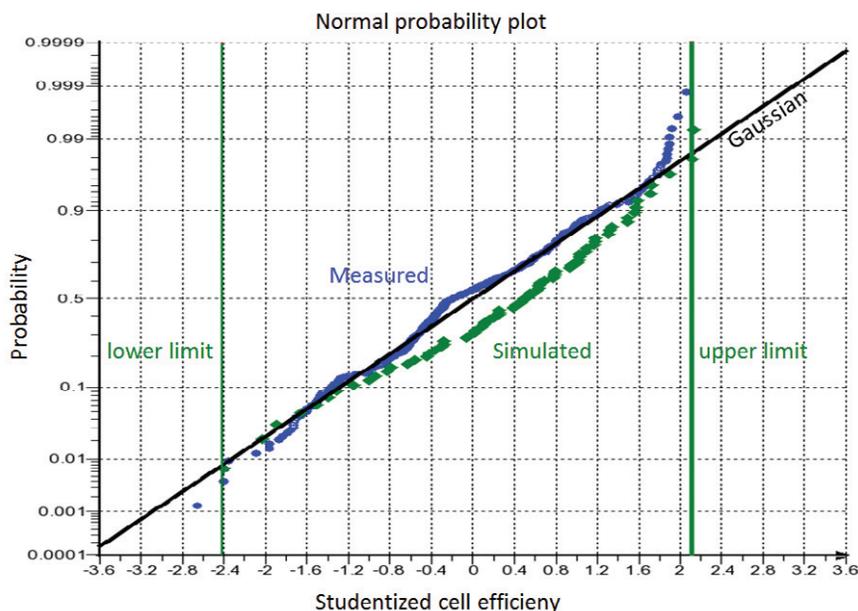


Fig. 3. Normal Probability Distribution of measured cell efficiency from mass production (circles), and simulated cell efficiency (diamonds) as compared to a Gaussian distribution (line)

5. Conclusion and Application

We introduced a new methodology, similar to established methods in integrated circuit design, based on a combined statistical and TCAD model. The principal dependencies are well reproduced by our statistical model based on the TCAD simulations. Additionally we have shown that the distribution of cell efficiency is well reproduced. This indicates that the variations observed in mass production are mainly caused by variations in bulk lifetime, metallization fraction, and lumped series resistance, and only to a lesser extent due to other variations. However, in our ongoing work, we extend the combined model with additional variations (e.g. the emitter doping profile, the base resistivity and varied carrier generation profiles). This leads to even more realistic description of the production cell parameter distribution.

This derived statistical model is used for optimization strategies for higher efficiency, smaller variations in cell parameters and improved yield in mass production.

Furthermore, we apply our methodology to advanced cell concepts. It allows the early consideration of production fluctuation in device simulation of advanced cell concepts, and therefore a realistic assessment of such concepts.

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