

ASSESSMENT OF INFLUENCING FACTORS ON LIFETIME-BASED DEFECT ANALYSIS

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ABSTRACT: Since most detection methods are not sensitive enough to detect and characterize recombination active defects in silicon lifetime spectroscopy is an important method in silicon photovoltaics. It is a powerful tool, that can determine the defect parameters E_t and k via the analysis of defect parameter solution surfaces. But despite being a crucial method there is no convention for the assessment of uncertainties. This work lines out a possible way to characterize the uncertainty of the method by a simulation of statistical noise onto lifetime curves following the Shockley-Read-Hall-statistics. The uncertainty analysis is done for one exemplary set of defect parameters. It outlines how prone to wrongful parametrization this method can be, if not conducted with great care. Thereby the suggested approach can act as a tool to decrease the uncertainty of the method by understanding, which influences are most crucial to control.

1 INTRODUCTION

One way to maximize solar cell efficiency, next to cell and module technological improvements, is the optimization of the carrier lifetime of the given material. Two prominent recombination channels that can be controlled are the surface recombination and the bulk lifetime. Improvements of the passivation schemes in recent years have minimized the surface recombination drastically. With passivation layers such as Tunnel-Oxide-Passivating contact (TOPCon) the impact of surface passivation on efficiency only shows on highest quality base material. The other adjustable recombination channel is recombination via defects in the wafer bulk. The bulk lifetime can be affected by defects that act as recombination centers according to the Shockley-Read-Hall (SRH) statistics [1, 2]. Oftentimes the defect concentrations are below the detection limits of most detection methods and lifetime measurements are the best method of detection. Such defect centers can then be identified by lifetime spectroscopy (LS). A common approach for analysis of defect parameters via LS is by means of the defect parameter solution surface (DPSS) [3].

In theory DPSS analysis is a powerful tool to determine the defect parameters of the limiting defects, as Rein has shown in the detailed elaborations in [3]. However, in reality, the obtained solution is rarely as distinct as desired. This is not surprising since there are a lot of factors affecting the analysis, e.g. statistical and systematical measurement uncertainties, the presence of multiple defect levels (from different impurities, different defect complexes or multivalent defects), and of course the influences of intrinsic recombination and surface recombination.

In spite of the importance, an error estimation of temperature- or doping-dependent injections dependent lifetime spectroscopy (TIDLS or N_{Dop} IDLS) has not been commonly used so far. This work intends to highlight the influences of different factors by analyzing their contributions to the uncertainty of determined defect parameters. In this way, we are able to evaluate what experimental criteria have to be met to justify drawn conclusions. It has to be mentioned, that this evaluation does not include sample processing or measurement errors, which could affect the measurements. It merely tries to estimate the uncertainty that the DPSS analysis inherently has. For evaluation of real data it might be necessary to consider the effects of processing and

measurement uncertainties on top of the considerations of this work. Yet another aspect that is not considered in this work is the comparability of defect parameters determined by IDLS with literature data, as discussed by Juhl et al. [4].

2 SIMULATION

In order to assess the uncertainty of the method a simulation was performed, where the influences of different error sources on the resulting DPSS analysis was evaluated. For illustration of the different effects the influences of a typical surface recombination, statistical noise and of the experimentally accessible injection range of the lifetime curve on a simple one-level SRH defect are presented in this work.

The final aim is to achieve error estimations for defect parameters extracted from real measurements. Therefore, we demonstrate an approach to estimate the uncertainty around a given defect parameter set by adding artefacts and restrictions until the analyzed curves resemble real measurement conditions. However, in order to track and easily understand the effects of the different contributions, the analysis of different cases - converging to real measurement conditions step by step - is helpful, as exemplarily demonstrated in the following:

Case A) Ideal simulated lifetime curves simulated via SRH statistics (defect specifications: $E_t = E_c - 0,3$ eV, $k = 10$, $N_t = 1 \times 10^{10}$, $\sigma_n = 4 \times 10^{-14}$) with four different doping densities (p-type doping, $N_{Dop} = (1 \times 10^{14}, 1 \times 10^{15}, 1 \times 10^{16}, 1 \times 10^{17})$ cm⁻³) on an injection range Δn of 10^{10} to 10^{20} cm⁻³. Surface recombination is simulated as surface limitation lifetime via a fixed saturation current J_0 term ($\tau_s = (e \cdot W \cdot n_i^2) / (J_0 \cdot (N_{Dop} + \Delta n))$) assuming a sample thickness of $W = 200$ μ m and $J_0 = 10$ fA/cm²).

In **Case B)** the simulated lifetime curves were superposed with 10% random noise at each data point. While this might not be the most appropriate representation for all measurement devices, it is an intuitive measure to bring fluctuation into the simulated curves and observe the effect onto the evaluation. Further Macintosh et al. have determined that the error of lifetimes measured with the Sinton Instruments Lifetime Tester is in the range of 10% [5].

The assumed injection density range for cases A) and B) covering ten orders of magnitude is far from a realistic range of experimental data. Therefore, the range was

restricted to Δn of 10^{14} to 10^{16} cm^{-3} for **Case C**). This range is typical for measurements with the Sinton Instruments Lifetime Tester that is common in photo voltaic research.

To analyze the simulated data, it was fitted with the linearization approach of Murphy et al. [6], as a single-level SRH defect is represented by a linear function within this parametrization. The simulated defect parameters were chosen in a way, that the general shape of the DPSS-curves change from pot-like to split curves for the given doping range [3], which yields a DPSS analysis with a distinct intersection, making the analysis more precise than in other cases. Intrinsic limitation was not added in the simulations as it is assumed that the intrinsic recombination is known well enough and can be sufficiently considered in the analysis of real-life data. For the assessment of the deviation within the DPSS plot for the cases B) and C), a set of 200 curves per case was simulated and individually analyzed. This yields a distribution of the resulting DPSS curves around the input value. The curves that represent the outer edges of the scattered results for each simulated sample are used to represent the upper and lower bounds of the solution area, creating a solution band.

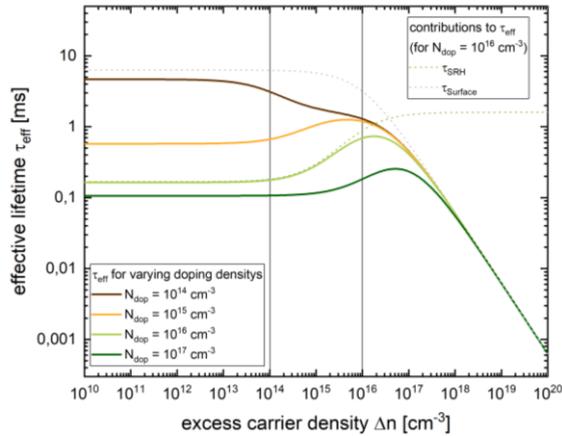


Figure 1: Simulated lifetime curves as described in case A). Defect specifications: $E_t = E_c - 0,3$ eV, $k = 10$, $N_t = 1 \times 10^{10}$, $\sigma_n = 4 \times 10^{-14}$, Surface parameters: $J_0 = 10$ fA, $W = 200$ μm . Exemplary SRH lifetime and surface lifetime for the sample with $N_{\text{Dop}} = 1 \times 10^{16}$ cm^{-3} are displayed as dotted lines. The vertical lines indicate the restricted range of the lifetime curves that is accessed in case C).

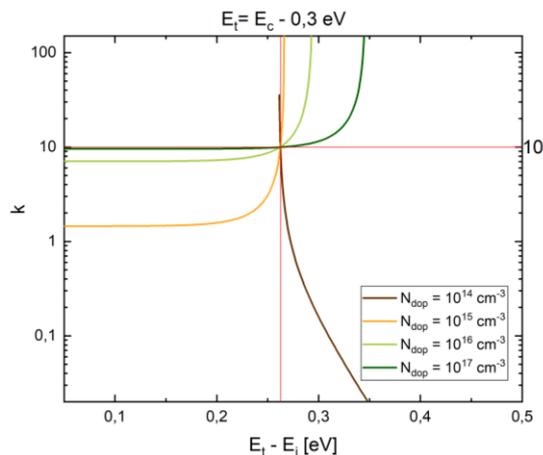


Figure 2: Defect parameter solution surface analysis for the case A). The red lines indicate the values of the input parameters that were used for simulation.

3 RESULTS AND DISCUSSION

Figure 1 shows the simulated lifetime curves for case A). For the doping density of $N_{\text{Dop}} = 1 \times 10^{16}$ cm^{-3} also the individual contributions of defect recombination and surface limitation are shown. Figure 2 presents the corresponding DPSS analysis. As expected from theory [3] the DPSS analysis results in two intersections (one per band gap half). For better visualization the figure only shows the intersection in the upper band gap half. It was derived in [3] that it should be possible to distinguish between the true and false intersection by a close examination of the intersections, since the true one is sharp and the false one is more dispersed. This approach is only realistic for ideal SRH curves and does not find application in practice; the band gap half thus should be determined otherwise. For the evaluation of case A) we observe a sharp intersection at the input parameters and the evaluation of the surface limitation performed on the basis of the Kane-Swanson method [7] (more details to the J_0 -determination will be published in an upcoming paper) gives the value of $J_0 = 9.9 \pm 0.1$ fA/ cm^2 . As expected, the ideal case results in the reproduction of the used defect parameters.

Figure 3 shows the DPSS evaluation for case B). The range of DPSS curves obtained for each simulated case is shown as a band between the DPSS curves representing the most extreme deviations. It is apparent that this evaluation does not provide one exact solution, but rather a diffuse solution area (i.e. the area where all bands overlap). The error estimation can be drawn from the variance of the scattering. The true defect parameters lie within the overlapping region and the determined J_0 range of 13 ± 5 fA/ cm^2 agrees well with the input value. A first conclusion is therefore that statistical noise alone does not impede the determination of correct defect parameters.

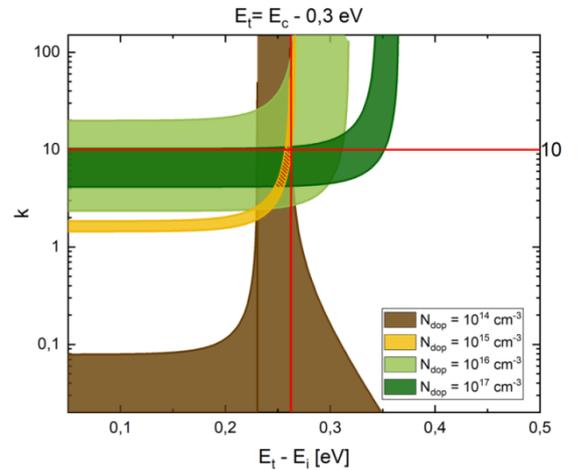


Figure 3: DPSS analysis for the case B). The DPSS curves for each sample are broadened by the statistical fluctuation of the analyzed curves and the respective results. The red lines indicate the value of the parameters that were used for simulation. The possible solution region is indicated by the area shaded in red.

However, in the next step we additionally restrict the investigated injection range to a more realistic scenario (case C), see Figure 4. As a result, the bands expand even further and the overlap area becomes too broad for meaningful parameter determination. It should be noted that the size of the DPSS bands correlates strongly to the chosen statistical noise and the chosen injection range, thus to give a proper estimation regarding one specific measurement method it is crucial to simulate the noise in an appropriate way. Another point showing the limits of this, close to realistic, data set is the result of the J_0 calculation, which does not yield a meaningful value: $J_0 = 64 \pm 101$ fA/cm². Of course, this outcome is not surprising since the accessible injection range does barely cover the region dominated by the surface limitation.

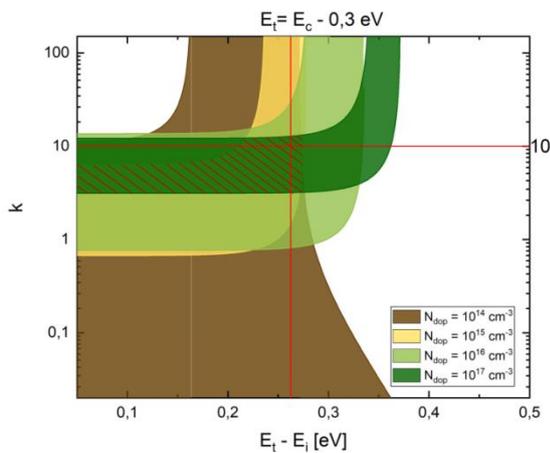


Figure 4: DPSS analysis for the case C). The DPSS curves for each sample are broadened by the statistical fluctuation of the analyzed curves and the respective results. The red lines indicate the value of the parameters that were used for simulation. The possible solution region is indicated by the area shaded in red.

During the evaluation of case C) an additional contributing factor was observed. Figure 5 shows the cropped lifetime curves in linearized form without added noise. Under experimental conditions some of these curves would likely be assumed to be linear and fitted with just one linear term. Particularly in an experiment featuring multiple samples (doping variation), where variations in the contamination between the samples cannot be excluded, one could thus be tempted to apply different fitting procedures for the different samples. In this example this could lead to a two-defect fit for the doping densities of $N_{Dop} = 1 \times 10^{14}$ and 1×10^{15} cm⁻³ and a one-defect fit for the doping densities of $N_{Dop} = 1 \times 10^{16}$ and 1×10^{17} cm⁻³. While this would be a reasonable choice based on the data (see illustration Fig. 5) this would result in wrong parameters. As shown in Figure 6, in that case the input parameters are no longer included in the overlapping area and the deviation from the actual parameters might well be more severe for other input combinations. Especially since the DPSS bands for the one-defect fit ($N_{Dop} = 1 \times 10^{16}$ & 1×10^{17} cm⁻³) are much narrower, which could easily be misinterpreted as a higher certainty of the determined parameter, whereas in reality this is only caused by the simpler fit with less degrees of freedom.

The general conclusion from this investigated step – which is a realistic one – therefore is that in order to

obtain a reliable parameter set when the measured injection range is restricted, it is necessary to decrease the measurement uncertainties as well as possible. Vice versa, we significantly increase reliability by pushing the investigated injection ranges as far as possible

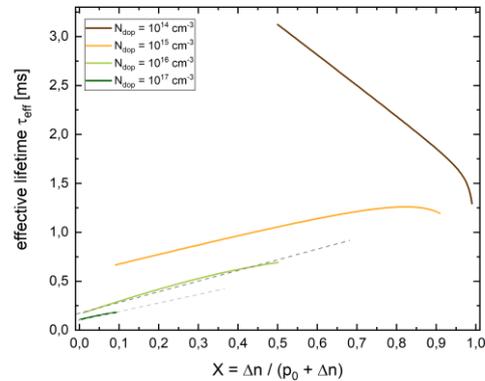


Figure 5: Effective lifetime curves in Murphy parametrization for an evaluation between the injection densities of $\Delta n = 1 \times 10^{14}$ cm⁻³ and 1×10^{16} cm⁻³. Ideal curves without the 10% scatter are displayed to enable an easier examination of the curvature. The dotted lines illustrated the misinterpretation conducted in the DPSS analysis shown in Fig. 6.

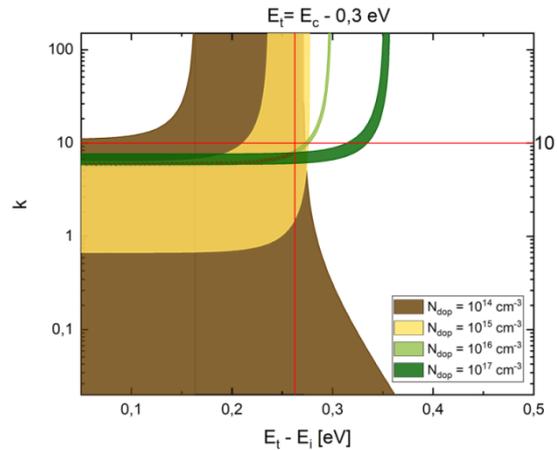


Figure 6: DPSS analysis for the case C), if the fitting is done with a one-defect fit for the doping density of $N_{Dop} = 1 \times 10^{16}$ & 1×10^{17} cm⁻³ and with a two-defect fit for the doping density of $N_{Dop} = 1 \times 10^{14}$ & 1×10^{15} cm⁻³.

4 CONCLUSION

The presented results demonstrate that the quality of DPSS analyses highly depends on the measurement conditions and on the assumptions on which the fitting procedure is based. The evaluation is showing that the error of DPSS analysis can be very broad, thus impeding a meaningful analysis - or even give wrong results.

Thereby this work shows one way to estimate the uncertainty of a given DPSS defect analysis and assess its reliability. Unfortunately, in application onto real data it is not easy or sometimes not possible at all to determine, whether the used assumptions are corrected or not, even if they are in general reasonable.

So far, this evaluation has been performed for exemplary combinations of SRH defect parameters and

surface recombination. To enable general uncertainty estimations – at least for some aspects - we are currently broadening this analysis to a multitude of defect combinations and surface limitations, with the goal to also cover the case of coexistence of multiple defects. Finally this approach will enable heuristic error estimation for certain influences on the lifetime spectroscopy. These results will be published in an upcoming paper.

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REFERENCES

- [1] W. Shockley and W. Read, “Statistics of the recombinations of holes and electrons,” *Phys. Rev.*, vol. 87, no. 5, pp. 835–842, 1952, doi: 10.1103/physrev.87.835.
- [2] R. Hall, “Electron-hole recombination in germanium,” *Phys. Rev.*, vol. 87, no. 2, p. 387, 1952, doi: 10.1103/PhysRev.87.387.
- [3] S. Rein, *Lifetime Spectroscopy: A Method of Defect Characterization in Silicon for Photovoltaic Applications*, 1st ed. Berlin, Heidelberg: Springer-Verlag Berlin Heidelberg, 2005.
- [4] Matthias Klaus Juhl, Friedemann D. Heinz, Gianluca Coletti, Fiore E. Rougier, Chang Sun, Tim Niewelt, Jacob J. Krich, Daniel Macdonald, Martin C. Schubert, “Insights on the electronic parameterisation of defects in silicon obtained from the formation of the defect repository,” *36th European Photovoltaic Solar Energy Conference and Exhibition*, 2019.
- [5] K. R. McIntosh, R. A. Sinton, and K. R. McIntosh, “Uncertainty in Photoconductance Lifetime Measurements that Use an Inductive-Coil Detector,” in *23rd EU PVSEC*, Valencia, 2008, pp. 77–82.
- [6] J. D. Murphy, K. Bothe, R. Krain, V. V. Voronkov, and R. J. Falster, “Parameterisation of injection-dependent lifetime measurements in semiconductors in terms of Shockley-Read-Hall statistics: An application to oxide precipitates in silicon: An application to oxide precipitates in silicon,” *J. Appl. Phys.*, vol. 111, no. 11, p. 113709, 2012, doi: 10.1063/1.4725475.
- [7] D. E. Kane and R. M. Swanson, “Measurement of the emitter saturation current by a contactless photoconductivity decay method (silicon solar cells),” in *18th IEEE Photovoltaic Specialists Conference Las Vegas*, Las Vegas, 1985, pp. 578–583.