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# Versatile simulation tool and novel measurement method for electrical characterization of semiconductors

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**Abstract.** A versatile numerical tool for the simulation of electrical properties of a semiconductor such as minority carrier lifetimes and photoconductivity as a function of defect parameters was developed. Unlike the SRH-model this tool enables to simulate e.g. different measurement conditions and even trapping effects. Contrary to the widely used simulation tool PC1D also non-steady state solutions can be obtained. Furthermore the novel contact less method MDP is presented. Using the example of iron determination the new possibilities arising from combining the novel simulation tool and the method MDP are shown. Simulations for different trapping densities and measurement conditions were executed and exemplary measurements of the trap density and the cross-over point of mc-Si wafers were performed. It was found, that the cross-over point and the sensitivity of iron determination at low level injections is effected by trapping and the chosen non- or steady state measurement conditions.

## Introduction

Most of the destruction free lifetime measurement methods like µPCD (microwave detected photoconductivity decay), QSSPC (quasi steady state photo conductance), CDI or the here presented method MDP suffer from trapping effects at low injection levels. The well-known SRH-theory, which is often used to describe lifetime measurements is not valid for trapping effects. Because of that the necessity for a better simulation tool arises, that can calculate precise measurement results for different trap densities. Besides that, it is known that the chosen measurement conditions can strongly influence the measured minority carrier lifetime, especially non-steady state methods like µPCD and steady-state methods like QSSPC can obtain very deviating measurement results. Unlike PC1D, the novel simulation tool is also able to simulate non-steady state results, so that an excellent evaluation of the different experimental methods mentioned above with respect to their applicability and validity of results is provided [1, 2] and a completely new access to trapping dynamics can be obtained. This was achieved by solving a generalized rate equation system for all possible transitions in the forbidden gap of a semiconductor.

Besides this novel simulation tool the contact less method MDP was applied. It e.g. enables measurements for an extremely wide range of injection levels, which comprises and exceeds that of other non- destructive methods as it is shown in figure 1. It is well suited for defect investigation and mapping of silicon wafers [3, 4].

Lifetime measurements before and after iron boron pair dissociation are a widely used method for iron determination in silicon wafers. Especially at multicrystalline silicon the trapping effect is very distinct and can influence this measurements. Using this as an example, the new possibilities arising from combining the novel simulation tool with the method MDP will be presented.

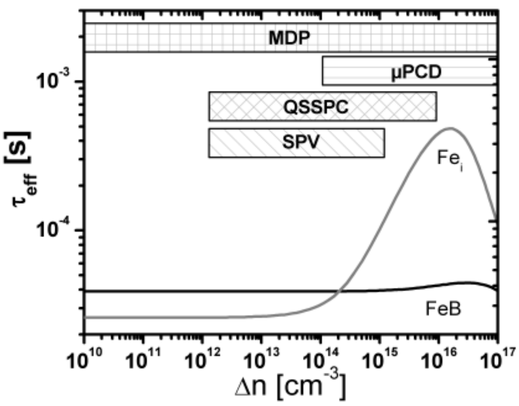


**Fig. 1:** Injection dependent lifetime curves for FeB and $Fe_i$ and injection ranges measurable by MDP, µPCD, QSSPC and SPV

## Methods

**Simulations by a rate equation system.** The novel numerical tool is based on a generalized rate equation system, which is solved for all possible transitions between the defect levels in the forbidden gap and bands of a semiconductor. The only approximation is, that no interactions between defect levels are included. This is a valid approximation, since the defect concentrations in silicon are typically low.

The applied rate equation system describes the time dependent change of carrier concentrations in the conduction and valence band ($\dot{n}, \dot{p}$), as well as in defect levels ($\dot{n}_T$).

$$\dot{n} = G_{BB}^{o} + G_{BB}^{th} + \sum_j \left(C_j - D_j\right) - U_{BB} - U_{Aug} \tag{1}$$

$$\dot{p} = G_{BB}^{o} + G_{BB}^{th} + \sum_j \left(F_j - E_j\right) - U_{BB} - U_{Aug} \tag{2}$$

$$\dot{n}_{Tj} = D_j + E_j - C_j - F_j \tag{3}$$

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In this equation system the optical and thermal generation rates ($G^{o}_{BB}, G^{th}_{BB}$), the band to band and Auger recombination rates ($U_{BB}, U_{Aug}$) and the carrier capture and emission rates from all defects ($C_j$, $D_j$, $E_j$, $F_j$) are included. The transition rates are described without any approximations, e.g. the emission rate of an electron is described with:

$$C = n_T(t)\cdot \sigma_n v_{th} \exp\left(-\frac{E_C - E_T}{k_B T}\right)\cdot \left[N_C - n(t)\right] \tag{4}$$

From the simulated time dependent carrier concentrations the photoconductivity can be calculated using the mobility model of DORKEL and LETURCQ [5]. The minority carrier lifetime can be extracted from the transient of the photoconductivity after $G_{opt}$ is set to zero. This lifetime evaluation technique is very similar to the used technique for transient methods like µPCD and MDP and guarantees simulated values, that should be in very good agreement with measurement results.
For the simulation of the cross-over point of FeB and $Fe_i$ as a function of trap density, the following defect model was used.

**Table 1:** defect model used for the simulations

| defect | $E_T$ [eV] | $\sigma_n$ [cm$^2$] | $\sigma_p$ [cm$^2$] | |
|---|---|---|---|---|
| FeB | $E_C$ - 0.26 | $2.5 \cdot 10^{-15}$ | $5.5 \cdot 10^{-15}$ | [6] |
| $Fe_i$ | $E_V$ + 0.39 | $3.6 \cdot 10^{-15}$ | $6.7 \cdot 10^{-17}$ | [6] |
| trap | $E_C$-0.35 | $1.0 \cdot 10^{-16}$ | 0 | |

**Measurements by microwave detected photoconductivity (MDP).** The novel method MDP is well suited for both, defect investigation by e.g. injection dependent minority carrier lifetime measurements, as well as mapping of wafer or even ingots for inline metrology. It exceeds his competitors µPCD and QSSPC in terms of sensitivity, resolution and speed.
The photoconductivity, which is closely related to the diffusion length is measured by microwave absorption during and after the excitation with a rectangular laser pulse. The high detection sensitivity enables the application also of weak laser pulses with unlimited duration facilitating experiments in non- or steady state. The effective minority carrier lifetime is extracted from the transient of the photoconductivity signal. The low level injection lifetime is strongly affected by trapping effects, similar to low injection QSSPC and µPCD measurements. The large range of injection levels (from $10^{10}\ldots10^{17}$) and the different measurement conditions, that can be measured with MDP enable a more detailed investigation of the cross-over point as a function of trap density.

**Estimation of trap density.** One of the major advantages of the MDP method is the possibility to measure minority carrier lifetime and steady state photoconductivity at the same time. With this ability it is possible to estimate the trap density by the slightly modified model of Hornbeck and Haynes [7]. This model includes only one trap level, so that the determined trap density is only an estimation.
If significant trapping effects occur the electron concentration in the conduction band no longer equals the hole concentration in the valence band, but the electrons in the conduction band plus in trap levels.
This leads to a higher hole concentration and hence to an increased photoconductivity.

$$\Delta\sigma = e\cdot\left[\Delta n(\mu_n + \mu_p) + \mu_p n_T\right] \tag{5}$$

In steady-state the trapped electron concentration is determined by

$$n_T = \frac{\Delta n \cdot N_T}{\Delta n + N_C \cdot \exp\left(\frac{-E_a}{kT}\right)} \tag{6}$$

Combining equation 5 and 6 leads to a fit function of the injection dependent steady state photoconductivity with which the trap density and its activation energy can be estimated.

Figure 2 shows an exemplary photoconductivity measurement at a mc-Si wafer, the fit-curve and the corresponding measured apparent lifetime.

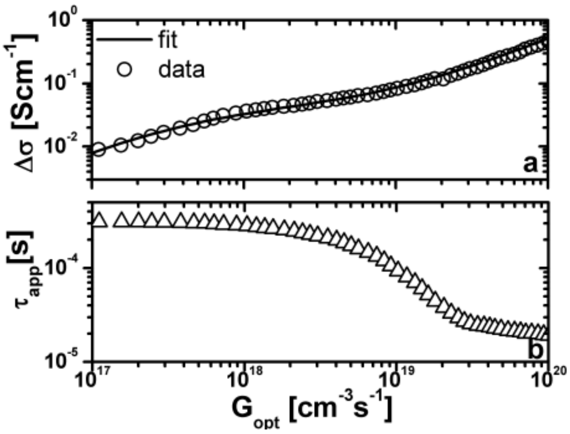


**Fig. 2:** Measured photoconductivity and fit curve versus $G_{opt}$ (a); apparent lifetime versus $G_{opt}$ (b); determined trap parameter: $N_T = 8 \cdot 10^{14}$ cm$^{-3}$, $E_A$ = 0.387 eV

### Experimental Details

Mc-Si wafers (156 x 156 mm) from different heights of an ingot with a resistivity of about 1 Ωcm and a surface passivation by silicon nitride film deposition were measured at room temperature with a 978 nm laser. Injection dependent lifetime and photoconductivity measurements were performed by MDP and the trap density was estimated. Afterwards the FeB pairs were dissociated with 50 flashes by a 1500 W flashlight and again injection dependent measurements were performed. The injection dependent measurements were executed with a 200 µs light pulse and the currently shortest light pulse possible at the MDP system (3 µs length), in order to compare steady state and non-steady state conditions. For steady state measurements the injection was calibrated with the part of the lifetime curve, which was dominated by Auger recombination. For non-steady state measurements it is more complicated, because strictly speaking the injection is not even defined for non-steady state. For this first measurements a pragmatic approach was used, where the injection was reduced by a constant factor, which was determined from simulations.

### Results and Discussion

The calibration factor for the iron determination, which is closely related to the cross-over point (COP) was investigated by simulations and measurements. Figure 3 presents the simulated apparent lifetime curves for FeB and $Fe_i$ for different trap densities and the resulting calibration factor C. For better clarity the reciprocal calibration factor is displayed.

This is a measure for the sensitivity of the iron measurement and hence becomes zero at the cross-over point.

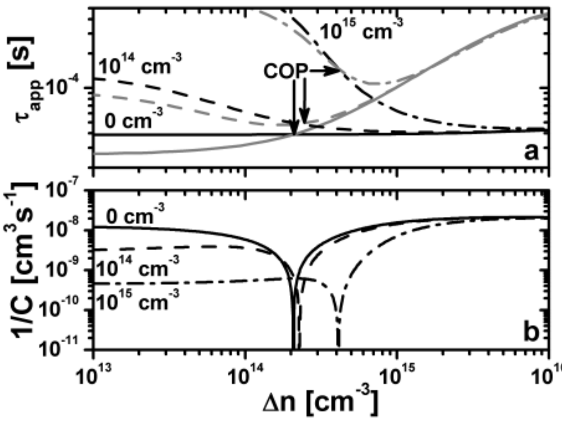


**Fig. 3:** Simulated apparent lifetime curves for FeB (black) and $Fe_i$ (grey) for three different trap densities (a); resulting reciprocal calibration factor versus injection (b)

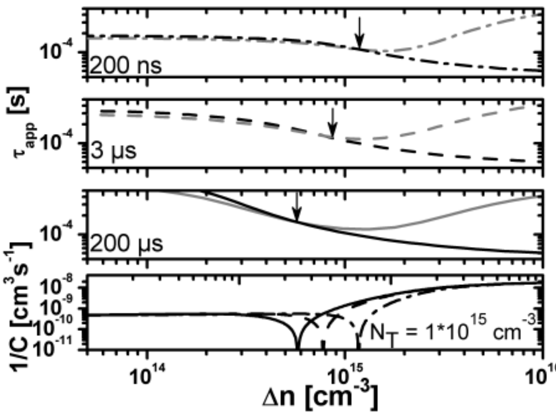


**Fig. 4:** Simulated apparent lifetime curves for FeB (black) and $Fe_i$ (grey) for three different laser pulse lengths; resulting reciprocal calibration factor versus injection

The simulation clearly shows, that the effective cross over point depends on the trap density. Because of the trapping effect both lifetime curves increase at low injections, which leads to a cross over of both curves at higher injection and to a smaller difference between the FeB and the $Fe_i$ curve at low injection. Consequently the reciprocal calibration factor also varies and the sensitivity at low injection decreases strongly with increasing trap density.

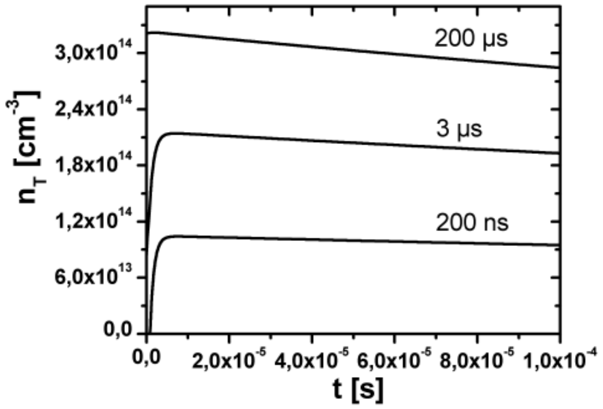


**Fig. 5:** captured electron concentration versus time after light has been switched off (t = 0 µs) for three different laser pulse length

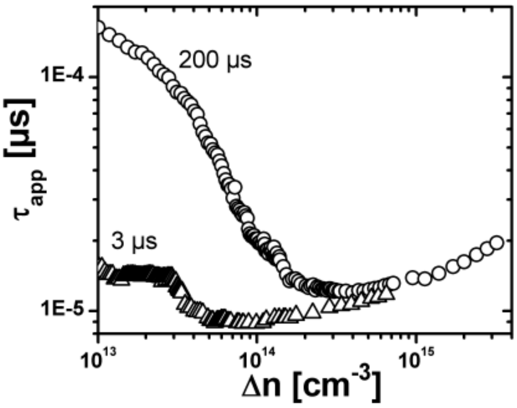


**Fig. 6:** Measured lifetime curves with 3 µs and 200 µs pulse length

Furthermore the applied lifetime measuring method has to be considered. The non-steady state method µPCD uses a very short light pulse during which no steady state is reached and hence the trap levels are not saturated completely. After the light pulse is switched off electrons and holes recombine and additionally carriers are trapped by the not saturated traps This effect leads to a faster depletion of the conduction band and an apparent smaller lifetime than with a steady state method [1]. In figure 5 the time dependent captured electron concentration for three different laser light pulse length is shown. Figure 3 displays the apparent lifetime curves for FeB and $Fe_i$ for different laser pulse length and an trap density of $1{*}10^{15}\,cm^{-3}$. The apparent increase of lifetime at very low injection levels is less pronounced with smaller laser pulse length, but the trapping effect starts at higher injections. Note again, that this does not always lead to an increase of the apparent lifetime, but can even lead to an decrease at higher injections. All in all these effects also cause a measured cross-over point at higher injection levels.

In figure 6 two by MDP measured lifetime curves with different laser pulse lengths are displayed. As expected the apparent lifetime with the non-steady state measurement conditions (3 µs pulse length) is smaller at low injection levels.

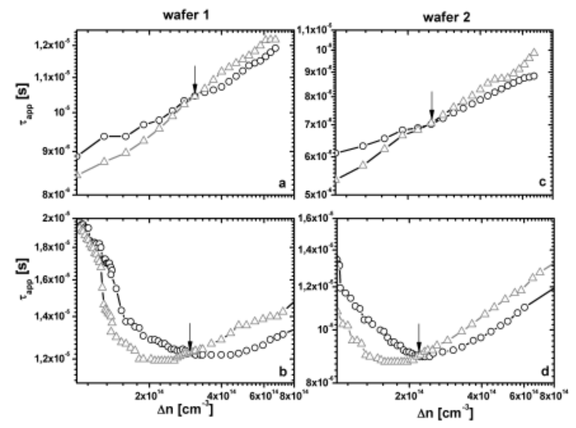


**Fig. 7:** Measured lifetime curves with 3 µs and 200 µs pulse length before (black) and after (gray) dissociating the FeB pairs

**Table 2:** Sample parameters

| | wafer 1 | | wafer 2 | |
|---|---|---|---|---|
| $\rho$ [$\Omega$cm] | 1.19 | | 1.35 | |
| $N_T$ [$cm^{-3}$] | 1.3 x $10^{14}$ | | 9.0 * $10^{13}$ | |
| $\Delta n_{COP}$ [$cm^{-3}$] (without traps) | 2.2 x $10^{14}$ | | 2.1 x $10^{14}$ | |
| $\Delta n_{COP}$ [$cm^{-3}$] (measured) | 3 µs<br>3.1 x $10^{14}$ | 200 µs<br>2.9 x $10^{14}$ | 3 µs<br>2.5 x $10^{14}$ | 200 µs<br>2.2 x $10^{14}$ |

Exemplary measurements of the cross-over point at two mc-Si wafer are displayed at figure 7. The measured injection levels for the cross-over point are clearly at an higher injection than the calculated values without trapping effect. Table 2 summarizes the measured sample parameters.
Keep in mind that the chosen defect model for the simulations is very simple and surface recombination is neglected, so that it can not be expected, that the measured lifetimes exactly fit the simulated values. However the effect is clearly evident in this first measurement results.

**Conclusions**

The novel numerical tool proofed to be a versatile tool for minority carrier lifetime simulations and clearly surpasses the possibilities of simple SRH simulations. It enables a completely new access to trapping effects, which evidently is very important especially when it comes to multicrystalline silicon. With the example of iron determination the practical use of such simulations could be shown.
Simulations and measurements demonstrated, that the measured cross-over point of iron detection is strongly dependent of the trap density and the measurement conditions, which is reflected in first experimental results. A measurement at non steady state leads to an even higher deviation from the cross-over point, but note that the injection is only an estimation for this case.
The novel method MDP proved to be well suited for injection dependent measurements of minority carrier lifetime and photoconductivity and offers the possibility of adjusting the measurement conditions to non-steady state or steady state measurements.
To summarize, combining the novel method MDP with the newly developed simulation tool, enables a more precise defect and measurement condition investigation and a completely new access to trapping dynamics.

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