INFLUENCE OF DEPTH DEPENDENT PROFILES ON CARRIER DENSITY MEASUREMENTS

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ABSTRACT:

Carrier density is a frequently examined parameter for silicon material characterisation. Besides the detection of the minority carrier lifetime under low injection conditions like QSSPC, CDI/ILM, and PL more advanced material characterisation methods are based on carrier density measurements. Although spatial resolution has been included in many measurement techniques, the depth dependence of the carrier profiles is typically neglected and homogeneous carrier profiles are assumed. This assumption, however, does not hold for many practical cases and may introduce significant systematic errors. In this work, analytical simulations show the expected errors quantitatively. Iron imaging is taken as an example to demonstrate the magnitude of the systematic error. A correction method is provided which accounts for the inhomogeneous carrier profiles.

1 INTRODUCTION

Carrier lifetime in silicon is dependent on injection level. For lifetime measurements carriers are typically generated optically from the front or back side which results in an inhomogeneous generation profile due to the photon absorption process. Lifetime measurement techniques like QSSPC [1] and ILM/CDI [2-4] are measuring an integral value over the thickness of a sample under test. The resulting lifetime is only correct if the carrier density is constant in good approximation or if the lifetime is not dependent on carrier density in the relevant range (i.e. low level injection conditions). Similar conditions apply for Photoluminescence (PL) [5] measurements where reabsorption has to be considered, too. In order to estimate the occurring errors when the conditions of low injection or homogeneous carrier profile are not fulfilled, carrier profiles are simulated for given recombination centres in the sample, surface recombination, and experimental conditions like the illumination spectrum. For small recombination lifetime, for example, i.e. small diffusion length of minority carriers, the carrier profiles are inhomogeneous even if no surface recombination occurs and will, in the limit case of infinitesimal lifetime, follow the shape of the generation profile.

This contribution deals with the effect of inhomogeneous carrier profiles on lifetime measurements. Measurements of the interstitial iron concentration are taken to exemplify the role of the systematic error which originates from inhomogeneous carrier profiles (see also [6]).

These profiles are calculated considering a continuity equation which includes an injection dependent recombination term $U(\Delta n(z))$ accounting for different and injection dependent recombination processes.

Together with appropriate boundary conditions, which take the surface recombination into account, carrier profiles can be calculated. From these profiles virtual measurement results are obtained which are, in the case of QSSPC or CDI/ILM, proportional to an integration of $\Delta n(z)$ over the thickness of the sample. In case of PL reabsorption has to be considered additionally. The simulated measurement results are then used to recalculate the interstitial iron concentration. A correction procedure is developed.

2 IRON CONCENTRATION IMAGING

Iron is a major contaminant in silicon for solar cells which commonly limits the performance of multicrystalline solar cells. In order to reduce its detrimental effect on the recombination lifetime and the cell performance the quantitative and spatially resolved detection of iron in silicon wafers at different process steps is very valuable.

Fe-imaging is a very specific and simple technique to detect the interstitial iron concentration quantitatively which consists of the interpretation of two lifetime measurements on the same sample under different conditions: One measurement is performed on an annealed sample where instead of interstitial iron only iron-boron pairs are present and a second measurement where the iron-boron pairs are completely decomposed. Since the defect properties such as energy level and capture cross section differ from one to the other state, differences in the measured recombination lifetime occur. The method has been applied to non-spatially resolved measurements [7].

Recently, spatially resolved lifetime measurements by means of photoluminescence [8] have been used for a spatially resolved iron detection. Quantitative maps of the interstitial iron concentration can be obtained (see Figure 1).



Figure 1: Quantitative imaging of interstitial iron (left) based on lifetime measurements before and after light soaking and recombination lifetime image on same sample of multicrystalline silicon (right).

3 SIMULATION OF CARRIER PROFILES AND INFLUENCE ON IRON DETECTION

3.1 Simulation of carrier profiles

Optically generated carriers can be described by the continuity equation. In the stationary case this reads for electrons in p-type silicon

$$D_n \frac{d^2 \Delta n(z)}{d z^2} + G(z) - U(z) = 0 , \qquad (1)$$

where D_n is the electron diffusion constant, G(z) is the generation rate and U(z) is the recombination rate. The generation rate for an optical irradiation with a spectral photon flux density $J_{ph}(\lambda)$ is given by

$$G(z) = \int \left(J_{ph}(\lambda) (1 - R(\lambda)) \right) \alpha(\lambda) \exp(-\alpha(\lambda) z) d\lambda \cdot (2)$$

 $R(\lambda)$ is the reflection coefficient of the sample surface and $\alpha(\lambda)$ is the absorption coefficient. The recombination rate is under low level injection (LLI) conditions with the LLI recombination lifetime τ_{LLI}

$$U(z) = \frac{\Delta n(z)}{\tau_{LLI}}.$$
(3)

Since in most practical cases LLI conditions are not fulfilled and lifetime is injection dependent we use expressions for the Shockley-Read-Hall recombination and Auger recombination instead of equation (3)

$$U(z) = U_{SRH,Fei/FeB}(\Delta n(z)) + U_{SRH,other}(\Delta n(z)) + U_{rad}(\Delta n(z)) + U_{Aue}(\Delta n(z))$$
(4)

Surface recombination is included by boundary conditions for the front and back side of the sample:

$$D_{n} \frac{d \Delta n(z)}{d z} \bigg|_{z=0} = S_{f} \Delta n(0);$$

$$D_{n} \frac{d \Delta n(z)}{d z} \bigg|_{z=d} = -S_{b} \Delta n(d)$$
(5)

 S_f and S_b are the surface recombination velocities at the front and back surface, respectively.

Equation (4) with boundary conditions (5) can be solved numerically. Comparison to PC1D simulations have shown good agreement. Figure 2 shows examples for calculated carrier profiles for interstitial iron respectively iron-boron pairs being present as the only contaminants at two different assumed iron concentrations.

3.2 Simulation of carrier lifetime measurements and discussion of systematic errors

Recombination lifetime measurement techniques such as QSSPC or CDI/ILM measure the integrated carrier density Δn_{mean} represented by the black lines in Figure 2. The mean lifetime τ_{eff} then results by dividing Δn_{mean} by the mean generation rate G_{mean} :

$$\tau_{eff} \left(\Delta n_{mean} \right) = \frac{\Delta n_{mean}}{G_{mean}} \,. \tag{6}$$

The iron concentration is typically deduced from such mean values. It is, up to now, not taken into account for the calculation of the iron concentration that the carrier density may vary several orders of magnitude from front to back side of the sample (see Figure 2).



Figure 2: Simulated carrier profiles for different interstitial iron concentrations with monochromatic front side illumination ($\lambda = 790$ nm at $J_{ph} = 5.1 \cdot 10^{17}$ cm⁻³s⁻¹ (2 suns)). Surface recombination and front side reflection have been neglected. The dashed lines indicate the integral value which would result from a QSSPC or CDI measurement, for example.

In order to estimate the systematic error of this effect simulations of carrier profiles with various iron concentration as interstitial iron or iron-boron pairs have been performed. The material quality has been assumed to be laterally homogeneous in order to demonstrate the pure depth effect on the systematic error. Virtual QSSPC and CDI/ILM measurements have been obtained by integrating the carrier profiles. If Photoluminescence measurements are simulated, reabsorption needs to be taken into account. The qualitative result, however, will not differ from the considered integral case.

From the simulated carrier density measurements corresponding lifetime values are calculated following equation (6).

The results of these measurements have then been used to recalculate the iron concentration. The deviation of the initially set concentration of interstitial iron from the recalculated value is expressed as

$$\sigma_{rel} = \frac{[Fe_{recalc}]}{[Fe_{initial}]} - 1 \tag{7}$$

and plotted as a function of the illumination intensity and the set iron concentration see Figure 3). Monochromatic irradiation with λ =790 nm, a base doping of 10¹⁶ cm⁻³, and a sample thickness of 200 µm as well as perfectly passivated surfaces have been assumed.



Figure 3: Systematic quantitative error of iron concentration measurements in dependence of illumination intensity and iron concentration.

In the simulation shown in Figure 3 iron is assumed to be the only recombinative defect, whereas Figure 4 shows the impact of a second defect which is assumed to be independent from injection and light soaking. As an example, a defect which limits the lifetime to $\tau = 30 \ \mu s$ is assumed.



Figure 4: Systematic quantitative error of iron concentration measurements in dependence of illumination intensity and iron concentration. A second defect with $\tau = 30 \ \mu s$ has been added to the simulation.

It can be deduced from Figures 3 and 4 that, although negligible for certain parameter constellations, systematic errors may be substantial. It can be stated that the influence of an additional recombination centre on the systematic error is rather weak. The black line in Figure 4 represents conditions where the simulated measurement signal is equal for interstitial iron and iron-boron pairs, i.e.

$$\int \Delta n_{Fei}(z) \, dz = \int \Delta n_{FeB}(z) \, dz \, \cdot \tag{8}$$

Parameter combinations around these values do not yield significant systematic errors but are subject to enormous statistical errors because of the minority carrier detection sensitivity. Left from this line systematic errors are very small.

If parameter combinations right of the black line in Figure 4 are chosen, large errors may occur which increase with illumination intensity. For very high iron concentration the systematic error decreases.

4 ORIGIN OF SYSTEMATIC ERROR

The origin of the large systematic error is evident when the injection dependent recombination lifetimes for Fei and FeB defect recombination are plotted and compared to different illumination levels (see Figure 5). As example an interstitial iron concentration of $1.6 \cdot 10^{13} \text{ cm}^{-3}$ has been chosen for the simulation. The black diagonal lines represent values of identical illumination intensity from 0.1 to 10 suns (0.255 to $25.5 \cdot 10^{17}$ photons cm⁻²s⁻¹). Below an illumination intensity of 0.5 suns low level injection conditions are fulfilled in good approximation such that the recombination lifetime is constant over the sample depth. For higher illumination conditions the Fe_i recombination lifetime in particular becomes injection dependent and, thus, differs significantly from surface to back side of the sample (cf. Figure 2). The integrated value which is obtained by a simulated lifetime measurement is not adequate to account for the non-linear characteristics of the lifetime curve.



Figure 5: Injection dependent lifetime curves for Fe_i and FeB. The black lines represent values of constant illumination intensity.

The impact of the systematic error on the measurement result as a function of iron concentration is illustrated in Figure 6. Three qualitatively different regions have been identified. In region I recombination is low due to the small iron concentration. The corresponding high lifetimes yields homogeneous carrier profiles which result in a small error. In region II moderate lifetime values cause significant systematic errors due to two reasons: (i) The carrier profile is less homogeneous and (ii) lifetime is strongly injection dependent. The systematic error for region III is small again although the carrier profile is very inhomgeneous. This observation is due to the applying low injection conditions where lifetime is independent on injection.



Figure 6: Systematic error of iron concentration measurements as a function of the interstitial iron concentration. Three characteristically different regions have been marked (see text for details).

The effect of the up to now neglected surface recombination has been studied in Figure 7. Within the simple approximation of equation (1) surface recombination would be expressed as an additional recombination path $1/\tau_{surface}$. Considering the depth dependence of Δn , however, the effect is fundamentally different as the following simulation will show. The boundary conditions (equation (8)) have been varied from S = 0 to $S = 10^7$ cm/s. For simplicity we have assumed S to be independent of injection with $S = S_f = S_b$.

As demonstrated in Figure 7 large values for the surface recombination velocity result in significant systematic errors which are not predicted by the approach of equation (1). The observed error originates from large inhomogeneities of the carrier profiles.



Figure 7: Simulation of the impact of surface recombination on the systematic error on iron concentration measurements. Large values of surface recombination velocities provoke significant systematic errors.

Finally, the role of the wavelength of the irradiation source is shown in Figure 8. Since photon absorption is strongly wavelength dependent, the carrier profile depends on the energy of the incident photons, in particular if the carrier lifetime is small. Larger wavelengths yield more homogeneous carrier profiles which lead to smaller systematic errors as it is demonstrated in Figure 8. Using larger wavelengths is thus beneficial for a reduction of the systematic error. However, experimental boundary conditions may require small wavelengths (e.g. for PL). QSSPC measurements are frequently performed with a polychromatic flash. A simulation assuming a measured flash spectrum has therefore been included to the simulations and is shown in Figure 8. The resulting errors are comparable to the results for wavelengths of 790 nm and 860 nm.



Figure 8: Systematic error on iron concentration measurements as a function of excitation wavelength. For comparison, a simulation with a QSSPC flash spectrum is included.

Although this study is focused on the inherent and thus unavoidable systematic error, the statistical error is discussed in this paragraph for comparison with the systematic error of Figure 4. Figure 9 shows the statistical error of the quantitative detection of interstitial iron. In this simulation a statistical measurement error of $\sigma_{meas} = 5\%$ for a single lifetime measurement has been assumed.



Figure 9: Quantitative statistical error of iron concentration measurement assuming $\sigma_{meas} = 5\%$ as error on a single lifetime measurement.

5 CORRECTION OF ERRONEOUS

MEASUREMENTS

Although inherent the systematic errors can be corrected under the assumption that iron is the lifetime limiting defect or if the injection dependence of other involved defects is known. In this case, carrier profile simulations for various iron concentrations as shown in paragraph 3.1 can be performed with respect to the properties of the sample, i.e. thickness, doping concentration, and surface recombination on front and back side. According to paragraph 3.2 simulated iron concentration measurements can be calculated as a function of the assumed iron concentration. An example is shown in Figure 10.



Figure 10: Correction functions for iron concentration measurements for various illumination intensities. The corrected iron concentration [Fe]_{corrected} can be obtained from the measured value [Fe]_{meas}.

This function may then be used as a correction for all measurements with the same set of material parameters, e.g. a set of similar samples. For spatially resolved techniques this correction is valid for every pixel of a measurement. Note that for very high illumination intensities the result may be ambiguous such that two different solutions are deduced.

If other defects in addition to iron have a significant influence on the recombination lifetime, the additional recombination is included in equation 4 and a correction function can be calculated. If these defects are not known in their nature and concentration the systematic error cannot be precisely compensated. In this case, however, injection dependent lifetime measurements with QSSPC, for example, may be used as approximation for the injection dependence of the recombination lifetime.

6 CONCLUSION

The accuracy of recombination lifetime measurements may be affected by inhomogeneous carrier profiles. As an example, the quantitative measurement of the interstitial iron concentration from lifetime measurements before and after light induced degradation has been analyzed.

It has been up to now subject to substantial systematic errors in some cases which originate from the

assumption of homogeneous carrier profiles. This work demonstrates by simulations that this effect may result in errors as large as a factor of two and more for realistic parameter constellations.

Two essential conclusions can be drawn from the calculations: (1) Conditions are specified where quantitative measurements are valid without correction and (2) a correction technique is presented for parameter constellations yielding significant systematic errors.

Using the presented simulations these errors can be corrected for a certain range of conditions if iron is the lifetime dominating defect or if the injection dependence of other defect recombination is known. As approximation we propose measurements of the effective injection dependence of the recombination lifetime. Light induced degradation based iron detection techniques with QSSPC, CDI, or PL may in this way be significantly improved.

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