

## IRON QUANTIFICATION IN CRYSTALLINE SILICON SOLAR CELLS FROM OPEN-CIRCUIT VOLTAGE MEASUREMENTS

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**ABSTRACT:** Iron contamination in crystalline silicon can be quantified with high sensitivity thanks to its peculiarity to switch between interstitial and dopant-paired form, each exhibiting specific recombination activity. Typically, this is done by an iso-injective comparison of effective excess carrier lifetimes with iron either being interstitial or paired form. Within this contribution it is shown by means of PC1D simulations that the procedure works for solar cells as well, exploiting that effective lifetimes can be calculated from  $V_{oc}$  data. Furthermore, it is shown that even a comparison of  $V_{oc}$ 's taken at a constant intensity, meaning differing injection, already allows for a good estimation of iron contamination. Using multiple intensities allows an even better quantification.

**Keywords:** characterization, iron, quantification, silicon solar cell, simulation

### 1 INTRODUCTION

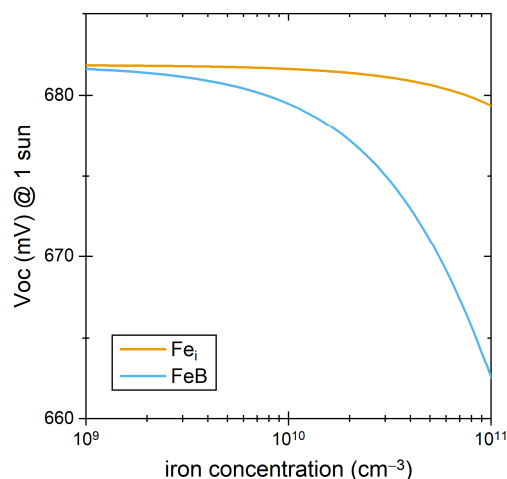
Iron is a common but unfortunately quite harmful contamination in crystalline silicon solar cells, even though it is often present 'only' in concentrations in the  $10^{10} \text{ cm}^{-3}$  range even after phosphorous gettering. Iron may exist in interstitial form ( $\text{Fe}_i$ ) or paired with acceptors like boron ( $\text{FeB}$ ) {or gallium ( $\text{FeGa}$ )}. In experiments iron can be easily toggled between  $\text{Fe}_i$  and  $\text{FeB}$  form {or  $\text{FeGa}$ } by short illumination steps and storage in darkness [1, 2]. Both forms are strongly recombination active, each affecting injection-dependent lifetime and, in consequence, solar cell performance (esp.  $V_{oc}$ ) in a specific way as shown in Fig. 1. In fact, this can be used for the quantification of iron in crystalline silicon [1, 2]. Typically, this is done by means of excess carrier lifetime spectroscopy on lifetime samples. Within this contribution, it is evaluated by means of PC1D simulations whether iron quantification is possible on cell level using open-circuit voltage ( $V_{oc}$ ) measurements only.

### 2 SIMULATION APPROACH

PC1D simulations [3] with well-known input data were used to evaluate the possibility to quantify iron contamination from  $V_{oc}$  measurements. The simulated PERC-like cell features a base doping of  $1 \times 10^{16} \text{ cm}^{-3}$  and a total front and rear surface saturation current density of  $110 \text{ fA/cm}^2$ . Series resistance is not of importance as the presented method relies on  $V_{oc}$  only. Iron contamination either in form of  $\text{FeB}$  or  $\text{Fe}_i$  was taken into account as Shockley-Read-Hall (SRH) defect with the well-known SRH parameters summarized in Table I. No other defect was assumed to exist. For ease of computation of generation rate, monochromatic illumination at 800 nm was used with an intensity of  $62 \text{ mW/cm}^2$  (photon-flux equivalent to 1 sun with AM 1.5g). As charge carriers fairly redistribute under open-circuit conditions, the deviating generation profile has a negligible impact on  $V_{oc}$ . The impact of iron contamination ranging from  $10^9$  to  $10^{11} \text{ cm}^{-3}$  on  $V_{oc}$  is shown in Fig. 1.

**Table I:** Defect-specific SRH parameters (from [2])

	$\sigma_n$ ( $\text{cm}^{-2}$ )	$\sigma_p$ ( $\text{cm}^{-2}$ )	E (eV)
$\text{FeB}$	$5 \times 10^{-15}$	$3 \times 10^{-15}$	$E_c - 0.26$
$\text{Fe}_i$	$4 \times 10^{-14}$	$7 \times 10^{-17}$	$E_v + 0.38$



**Figure 1:** Impact of iron either in interstitial form or paired to boron on the open-circuit voltage of PERC-like solar cell.

### 3 DATA ANALYSIS APPROACH

As pointed out by Kerr et al. [4], mass action law allows to translate pn-junction voltage (or  $V_{oc}$ ) into an excess charge carrier density  $\Delta n$  according to

$$n \cdot p = \Delta n^2 + \Delta n \cdot (n_0 + p_0) + n_0 p_0 = n_i^2 \cdot \exp\left(\frac{qV_{oc}}{kT}\right)$$

where  $n$  and  $p$  are total electron and hole densities while  $n_0$  and  $p_0$  denote electron and hole equilibrium densities,  $n_i$  the effective intrinsic carrier density and  $kT/q$  the mean thermal energy.

With known generation rate  $G$ , an effective lifetime  $\tau_{eff}$  can then be calculated according to

$$G \cdot \tau_{eff} = \Delta n$$

Hence,  $V_{oc}$  may be converted to  $\tau_{eff}$  valid at a certain injection  $\Delta n$ . In this context it is important to note that a difference in  $V_{oc}$  (Fig. 1) implies different injection  $\Delta n$ .

Effective lifetime can be approximated as the sum of inverse lifetimes related to iron ( $\text{FeB}$  or  $\text{Fe}_i$ ) and a non-iron related background ( $\tau_{bg}$ ).

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_{bg}} + \frac{1}{\tau_{\text{FeB}}} + \frac{1}{\tau_{\text{Fe}_i}} = \frac{1}{\tau_{bg}} + f_{\text{FeB}}[\text{FeB}] + f_{\text{Fe}_i}[\text{Fe}_i]$$

where the different recombination activity of  $\text{FeB}$  and  $\text{Fe}_i$

is captured by the known specific pre-factors  $f_{\text{FeB}}$  and  $f_{\text{Fei}}$  (following from SRH theory with parameters from Tab. I), and where the iron related lifetime components scale inversely with the respective concentrations  $[\text{FeB}]$  and  $[\text{Fei}]$ . Total iron concentration  $[\text{Fe}]$  resembles the sum  $[\text{FeB}] + [\text{Fei}]$ . In this context, it is important to note that FeB or Fei form may be toggled almost completely by storage in darkness (FeB forms) and illumination steps (FeB splits) so that either  $[\text{FeB}] = [\text{Fe}]$  or  $[\text{Fei}] = [\text{Fe}]$  while  $\tau_{\text{bg}}$  remains the same. If some iron does not switch its form or is clustered, it becomes part of the unchanged background. Insofar,  $[\text{Fe}]$  relates only to the part of iron toggled between FeB and Fei.

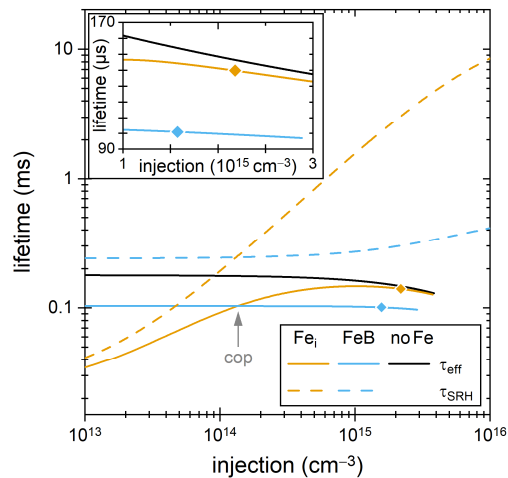
Solving the above equation system with either  $[\text{FeB}] = [\text{Fe}]$  or  $[\text{Fei}] = [\text{Fe}]$  yields

$$[\text{Fe}] = \frac{\left( \frac{1}{\tau_{\text{eff,Fei}}} - \frac{1}{\tau_{\text{eff,FeB}}} \right) - \left( \frac{1}{\tau_{\text{bg,Fei}}} - \frac{1}{\tau_{\text{bg,FeB}}} \right)}{f_{\text{Fei}} - f_{\text{FeB}}}$$

where all quantities with index FeB refer to the system with iron in the paired form and all quantities with the index Fei refer to the system with iron being in interstitial form. However, as mentioned earlier, a difference in  $V_{\text{oc}}$  occurring in iso-generative conditions (Fig. 1) implies a difference in injection  $\Delta n$  so that the quantities in the above equation refer to different injections:  $\Delta n_{\text{FeB}} \neq \Delta n_{\text{Fei}}$ , and background lifetime (even though unchanged) is not the same:  $\tau_{\text{bg,FeB}} \neq \tau_{\text{bg,Fei}}$ .

The situation is exemplarily shown in Fig. 2 for an iron contamination of  $5 \times 10^{10} \text{ cm}^{-3}$  where the effective lifetimes at  $V_{\text{oc}}$  in the FeB and Fei state are highlighted. As depicted in more detail in the inset, background lifetime is not constant in this injection range, implying that the background difference term does not cancel out and that  $[\text{Fe}]$  cannot be calculated from the change in  $\tau_{\text{eff}}$  due to a lack of information on the injection-dependence of  $\tau_{\text{bg}}$ .

In the following, it is discussed what this lack of information in iso-generative conditions means for the quantification of iron contamination.



**Figure 2:** Injection-dependent effective lifetimes and iron-related components with  $5 \times 10^{10} \text{ cm}^{-3}$  iron in FeB or Fei form (or absent for reference). The lifetimes calculated from  $V_{\text{oc}}$  are highlighted. Inset in linear scale.

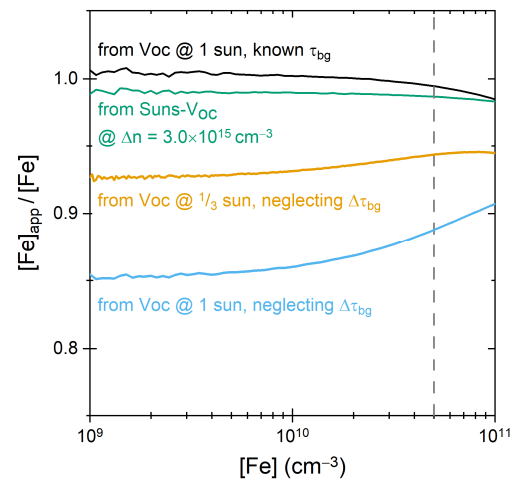
## 4 DISCUSSION

In principle, it would be better to adapt illumination intensity so that  $V_{\text{oc}}$  and thus  $\Delta n$  in the FeB and Fei state match and the background lifetime difference term in the above equation cancels out. In reality this would mean to measure  $V_{\text{oc}}$  not just at one intensity but rather in a certain intensity range. Or in other words, to use Suns- $V_{\text{oc}}$  measurements and select iso-injective conditions for analysis. As can be seen in Fig. 3, the corresponding green line yields reasonable results close to unity. Note that the exact result of the Suns- $V_{\text{oc}}$  analysis depends to some degree on the chosen injection level.

However, a Suns- $V_{\text{oc}}$  measurement might not be available. Hence, what does the iso-generative change in  $V_{\text{oc}}$  tell about the iron contamination?

The advantage of simulation is that background is well-known from simulation without iron contamination. Hence, the above equation may be used with this knowledge to evaluate whether the iso-generative approach works or not. As can be seen in Fig. 3, the corresponding black line is fairly close to unity as well, demonstrating that the above equation describes the situation correctly. But without any available knowledge on background lifetime, this approach is not viable in reality.

One possible approach is to simply neglect the change in background lifetime so that the background difference term cancels out even though this is obviously not true in the shown example (inset of Fig. 2). As can be seen in Fig. 3, this results in a certain underestimation of up to 15% (for 1 sun). Shifting the analysis to lower intensities like 1/3 sun yields an even better estimation of iron contamination. The reason behind this is that an analysis at lower intensity shifts  $V_{\text{oc}}$  to lower injection where background lifetime (black line in Fig. 2) flattens out so that the background difference term loses importance. The same happens in Fig. 3 for higher iron contamination which imply lower effective lifetimes and thus lower injection as well.



**Figure 3:** Ratio of apparent  $[\text{Fe}]_{\text{app}}$  and known iron contamination  $[\text{Fe}]$  evaluated across the assumed iron contamination range for different approaches calculated from the  $V_{\text{oc}}$  values shown in Fig. 1. The gray dashed line marks the situation from Fig. 2.

## 5 CONCLUSION AND OUTLOOK

Considering the simplicity of the approach – just a  $V_{oc}$  measurement before and after splitting of FeB and some calculations – neglecting the change in background lifetime seems a viable approach for the estimation of iron contamination on cell level.

An in-depth analysis of the presented approach including the impact of doping and a thorough error analysis is published elsewhere [5]. It is furthermore elaborated how the combination of  $V_{oc}$  measurements taken at different intensities can eliminate the lack of information on background lifetime leading to higher accuracy in the quantification of iron contamination on cell level [5].

## REFERENCES

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