Choosing the best silicon material parameters for different solar cell architectures

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Abstract

In a recent publication, we presented a comprehensive simulation study of industrially relevant solar cell architectures for an optimal material parameter choice, where the Shockley-Read-Hall lifetime was varied in the range of several microseconds to milliseconds with the assumption $\tau_n \approx \tau_p$. In the here presented investigation we focus on the influence of different impurities on the optimal doping concentration, taking into account more realistic (symmetric or asymmetric) behaviors of the lifetimes $\tau_n$ and $\tau_p$. Therefore, we present an application example of our recently published simulation study, where two different iron defects (iron boron pairs and interstitial iron) are implemented in different $p$-type silicon solar cells (Al-BSF, AlB-BSF and PERT). It is shown that the optimal doping concentration not only depends on the cell architecture, but that the device limiting impurity also plays an essential role.

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1. Introduction

The choice of the right silicon material, regarding quality and resistivity, is an issue of cell efficiency and production costs. There is always a tradeoff between these two criteria. Therefore, in a recent publication, we presented a comprehensive simulation study of industrially relevant solar cell architectures for an optimal material parameter choice [1]. The following different cell architectures have been investigated: Al-BSF, PERL, and PERT.

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We extensively investigated the cell performance dependent on the base material parameters by means of the Shockley-Read-Hall (SRH) lifetime and the base resistivity. Both parameters were treated independently to generate a fundamental understanding of the relevant dependencies by investigating the cell performance ($j_{SC}$, $V_{OC}$, $FF$ and $\eta$), the saturation current density $j_0$, and performing a detailed fill factor analysis ($pFF$ and $FF$) and a current density loss analysis.

In this work we will discuss a more specific issue where our models and the generated theoretical understanding can be applied for the investigation of specific cell concepts and materials limited due to distinct impurities. For simplicity reasons we will assume a material, which is limited only by one or two different impurities. By performing a detailed defect analysis of a certain solar cell and implementing the resulting defect configuration in our simulation the here presented method can be applied to determine the optimal doping concentration for distinct combinations of cell concepts and base materials.

As iron is one of the most important metallic impurities in silicon materials for photovoltaic application, we will focus on cell concepts featuring p-type base material and the contamination with iron, more precisely with (i) interstitial Fe (Fe$_i^+$) and (ii) interstitial iron-substitutional boron pairs (FeB). There is a permanent transformation of FeB to Fe$_i^+$ and B$^-$ and vice versa, which depends amongst other things on the temperature and the boron concentration [2]. Also, the transformation of FeB to Fe$_i^+$ and B$^-$ can be easily achieved by strong illumination [2, 3]. In our showcase we will focus on the ideal cases, where recombination in the silicon occurs either solely due to FeB or Fe$_i^+$.

2. Simulation setup and parameters

2.1. Cell architectures and models

All simulations presented in section 3 were performed using Sentaurus Device [4]. A schematic view of the cell concepts investigated as part of this work is shown in Fig. 1. The Al-BSF cell concept (a) is simulated in 2D, whereas the PERT structure (b) is simulated in 3D due to its rear point contact. Since front and rear pitch differ for the PERT structure, the front of the solar cell is simulated via a transparent electrode and an effective surface recombination velocity (compare Ref. [5]). For further details on the cell geometries please refer to Refs. [1, 6].

![Fig. 1. Schematic view of an (a) Al-BSF (also AlB-BSF) and a (b) PERT solar cell investigated in this simulation study.](image)

Some global assumptions have been made, in order to make the simulations of the different cell concepts comparable. A wafer thickness of 160 µm is assumed for both concepts as well as an optical shading of 4% and an external series resistance of 0.3 Ω cm$^{-2}$ for fingers and busbars. Also the cell geometries and all diffusions and contacts are kept constant and are not optimized individually for each base doping concentration.

2.2. Defect recombination parameters

There are two different ways to implement a SRH defect in Sentaurus Device:

(i) by activating SRH recombination in the physics section of the corresponding material and defining the SRH lifetimes $\tau_{n0}$ and $\tau_{p0}$ according to a SRH parameterization in the parameter file, or
(ii) by implementing Traps in the material and specifying the energetic position in the band gap as well as the cross-sections for electrons and holes.

Table 1. Defect parameters for FeB and Fei impurities. The cross-sections \( \sigma_n \) and \( \sigma_p \) are generally valid, whereas the lifetimes \( \tau_0 \) and \( \tau_0 \) were calculated exemplarily for a defect concentration of \( 2.5 \times 10^{11} \text{ cm}^{-3} \) and using a thermal velocity of \( 1 \times 10^7 \text{ cm s}^{-1} \).

<table>
<thead>
<tr>
<th>Defect</th>
<th>( E_C - E_{\text{trap}} ) [eV]</th>
<th>( \sigma_n ) [cm(^2)]</th>
<th>( \sigma_p ) [cm(^2)]</th>
<th>( \tau_0 ) [s]</th>
<th>( \tau_0 ) [s]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fei</td>
<td>0.745</td>
<td>4.0 \times 10^{-14}</td>
<td>7.0 \times 10^{-17}</td>
<td>1.0 \times 10^{-3}</td>
<td>5.7 \times 10^{-3}</td>
<td>MacDonald et al., Appl. Phys. Lett., 2006, 89, 142107 [3]</td>
</tr>
</tbody>
</table>

Both implementations have been tested using the parameters listed in Table 1. The results for both methods differ quantitative but the simulated trends are in good agreement. The deviation occurs due to the fact that method (i) only accounts for the SRH recombination, whereas by actually implementing traps (ii) the occupation and the space charge stored on traps are explicitly taken into account as well [4]. Therefore in the further simulations we applied method (ii).

![Fig. 2. Effective lifetimes of p-type silicon for (a) for FeB pairs (\( c_{\text{FeB}} = 2.5 \times 10^{11} \text{ cm}^{-3} \)) and (b) interstitial iron (\( c_{\text{FeI}} = 2.5 \times 10^{11} \text{ cm}^{-3} \)) based on the parameterizations for \( \tau_0 \) and \( \tau_0 \) listed and referenced in Table 1.](image)

The effective SRH lifetime \( \tau_{\text{eff}} \) dependent on the excess carrier density \( \Delta n \) can be calculated with

\[
\tau_{\text{eff}} = \frac{\tau_p \left( n_0 + n_1 + \Delta n \right) + \tau_n \left( p_0 + p_1 + \Delta n \right)}{n_0 + p_0 + \Delta n}
\]  

(1)

where \( n_0 \) and \( p_0 \) are the electron and hole concentrations in thermal equilibrium according to the \( n- \) and \( p- \) type doping concentrations and with

\[
n_1 = n_{\text{t,eff}} \exp \left( \frac{E_{\text{trap}}}{kT} \right)
\]  

(2)
The resulting effective lifetimes based on Eqs. (1) – (3) with $\tau_{e0}$ and $\tau_{p0}$ of Table 1 for a defect density of $c = 2.5 \times 10^{11} \text{ cm}^{-3}$ and using a thermal velocity of $1 \times 10^7 \text{ cm s}^{-1}$ are plotted in Fig. 2.

As expected from the cross-sections $\sigma_n$ and $\sigma_p$ in Table 1 FeB shows a rather symmetric behavior for the effective lifetime over the entire plotted excess carrier range, whereas Fe$_i$ shows a more asymmetric behavior especially for high base resistivity materials.

3. Simulation results

3.1. Influence of the trap concentrations

To demonstrate the influence of the impurity concentration on the cell performance dependent on the base doping we plot the efficiency $\eta$ over the base resistivity for an Al-BSF cell for different FeB concentrations $c_{\text{FeB}}$ in Fig. 3. We use FeB to demonstrate the effect of the trap concentration, due to its symmetric lifetime behavior. Therefore, the influence of $c_{\text{FeB}}$ presented in Fig. 3 is not altered due to lifetime effects.

The upper efficiency limit corresponding to a simulation without SRH defects is given by the dotted, blue line in Fig. 3a. Without SRH recombination in the bulk material a high base resistivity (low base doping) is beneficial to achieve high conversion efficiencies. This is due to an improved $j_{\text{SC}}$, which is shown in the topmost graph of Fig. 3b, and is a result of an improved high-low-junction for the lower base doping (compare also Ref. [1]). It is also shown that the $j_{\text{SC}}$ is mainly independent of the applied defect concentration. With increasing $c_{\text{FeB}}$ the $V_{\text{OC}}$ is reduced due to SRH recombination (Fig. 3b, middle), which also reduces the cell efficiency. This effect is less pronounced for the low base resistivity material, since a higher doping ensures a sufficiently high free carrier concentration, which
results in a higher $V_{OC}$. Additionally a $FF$ drop with increasing base resistivity can be observed in the lowermost graph of Fig. 3b. This $FF$ drop is actually a $pFF$ drop (compare Ref. [1]), and originates from injection dependent recombination. Therefore, the $FF$ drop is more pronounced for high defect concentrations similar to the $V_{OC}$.

Consequently, the maximum of the cell efficiency shifts towards lower base resistivities with increasing FeB concentration. For $c_{FeB} = 2.5 \times 10^{11} \text{ cm}^{-3}$ the maximal efficiency is achieved with a base resistivity of around 1 $\Omega$ cm.

3.2. FeB vs. Fe$_i$

For the comparison of the influence of different iron impurities (FeB and Fe$_i$) we chose a relatively high trap concentration of $2.5 \times 10^{11} \text{ cm}^{-3}$ in order to see significant effects of the different impurities. But it has to be emphasized that a concentration of $2.5 \times 10^{11} \text{ cm}^{-3}$ is quite realistic in industrial application, for example for multi-crystalline silicon. Also we want to emphasize that the here presented results are a showcase considering only one single defect for SRH recombination. In reality there is a variety of different defects responsible for SRH recombination. In order to perform a realistic simulation detailed characterization of the silicon material is needed to identify the relevant defects. The here presented showcase has the purpose to sensitize the reader to the influence of different impurities on the optimal doping concentration.

In Fig. 4 we plot the cell efficiency for three different solar cells (Al-BSF, AlB-BSF and PERT) over the base resistivity for $c_{FeB} = 2.5 \times 10^{11} \text{ cm}^{-3}$ (black) and $c_{Fe_i} = 2.5 \times 10^{11} \text{ cm}^{-3}$ (red). Both, the black and the red curves, obviously show a totally different behavior.

![Fig. 4](image.png)

Fig. 4. Cell efficiency for different cell structures (different lines) for different impurities of the same concentration $c_{FeB} = 2.5 \times 10^{11} \text{ cm}^{-3}$ (black) and $c_{Fe_i} = 2.5 \times 10^{11} \text{ cm}^{-3}$ (red) plotted over the base resistivity.

As already discussed in Fig. 3 the Al-BSF cell (filled symbols) in this configuration has a maximal efficiency at a base resistivity of around 1 $\Omega$ cm. For more advanced cell structures, here an AlB-BSF (open symbols) and a PERT cell (symbols with crosses), the overall efficiency increases, and the maximum of the efficiency curve shifts towards lower base resistivities (1). There are different reasons for this. One is that the influence of the base recombination becomes more significant when the surface recombination is reduced and therefore it is essential to ensure a
significantly high carrier concentration in the base material. Another is the reduced influence of an increasing $j_{\text{sc}}$ with lower doping concentration, since the high-low-junction is generally improved by implementing a higher doped BSF.

For the material solely limited due to the Fe$_i$ defect we distinguish between two resistivity regimes: (a) a low resistivity regime below $1 \ \Omega \ \text{cm}$ and (b) a high resistivity regime above $1 \ \Omega \ \text{cm}$. For low resistivities (a) The effective lifetime for Fe$_i$ is also constant over a large excess carrier range (compare Fig. 2b, solid red line), comparable to the effective lifetime of FeB (black, for all resistivities). Therefore, in this regime the efficiency curves of the different cell concepts show a similar behavior as for the FeB defects (2.a). This changes completely in the high resistivity regime (2.b). Here the asymmetric behavior of the effective lifetime for Fe$_i$ becomes the dominant influence. Due to a fast increasing lifetime curve for the high resistivity material at already relatively low excess carrier densities (compare Fig. 2b, dotted line) the cell efficiency extremely increases for high resistivity materials.

Again, we want to emphasize that the here presented results are just a showcase. Nevertheless, we have pointed out, how important it is to identify and consider the specific device limiting defects.

3.3. Additional lateral current flow effects - PERT vs. PERL

In the previous simulations, for the sake of simplicity, we only compared solar cell structures with a quasi-one-dimensional current flow in the base material: in the Al-BSF cells due to the full-area rear contact, and in the PERT cell due to the full-area rear diffusion. In Fig. 5 we compare the simulation results of the PERT structure for Fe$_i$ impurities with $c_{\text{Fei}} = 2.5 \times 10^{11} \ \text{cm}^{-3}$ (circles) with a PERL solar cell with the same defect configuration (stars).

Both structures show a similar behavior for low base resistivities. But in contrast to the efficiency of the PERT structure, which further increases for very high base resistivities for the simulated defect configuration, the efficiency of the PERL structure has a distinct maximum below a base resistivity of $10 \ \Omega \ \text{cm}$. For base resistivities $\geq 10 \ \Omega \ \text{cm}$ the (PERL) cell architecture becomes dominant for the cell performance again. Due to the lateral current flow component in the PERL structure, the $FF$ drops significantly for the high resistivity material due to a strong
increase of the series resistance (compare Ref. [1]). This again highlights the importance for an optimal material parameter choice dependent on individual cell architectures and the distinct device limiting impurities and underlines the complexity of this task.

4. Conclusion

We have demonstrated that for the determination of the optimal doping concentration not only the cell architecture but also the device-limiting impurities play a crucial role. Therefore, for optimizing the doping concentration via device simulation for a distinct combination of cell architecture and silicon base material a detailed characterization of the silicon material and the relevant impurities is essential for reliable simulation results. Another aspect which has not yet been taken into account is the interdependence of optimizing the doping concentration and optimizing the cell geometries. This also has to be considered when applying the presented approach on a distinct combination of cell architecture and base material. This underlines how complex the task of choosing the optimal base material parameters is and how many influences and parameters have to be considered. Therefore, device simulation is the best approach to tackle this challenging task.

References