Improved parameterization of Auger recombination in silicon

A. Richter\textsuperscript{a,*}, F. Werner\textsuperscript{b}, A. Cuevas\textsuperscript{c}, J. Schmidt\textsuperscript{b}, S.W. Glunz\textsuperscript{a}

\textsuperscript{a}Fraunhofer Institute for Solar Energy Systems (ISE), Heidenhofstr. 2, 79110 Freiburg, Germany
\textsuperscript{b}Institute for Solar Energy Research Hamelin (ISFH), Am Ohrberg 1, 31860 Emmerthal, Germany
\textsuperscript{c}Research School of Engineering, The Australian National University, Canberra, ACT 0200, Australia

Abstract

Accurate modeling of the intrinsic recombination in silicon is important for device simulation as well as for interpreting measured effective carrier lifetime data. In this contribution we study the injection-dependent effective carrier lifetime applying advanced surface passivation techniques based on Al\textsubscript{2}O\textsubscript{3} or SiN\textsubscript{x}. We show that in some cases the measured lifetime data significantly exceeds the previously accepted intrinsic lifetime limit proposed by Kerr and Cuevas [1]. To verify our measurements we independently perform lifetime measurements with different measurement techniques in two different laboratories. Based on effective lifetime measurements we develop an advanced parameterization of the intrinsic lifetime in crystalline silicon at 300 K as a function of the doping density and the injection level, which accounts for Coulomb-enhanced Auger recombination and Coulomb-enhanced radiative recombination.

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1. Introduction

Auger recombination processes in semiconductors are band-to-band processes where the excess energy – set free during the recombination of an electron and a hole – is transferred to a third charge carrier. As crystalline silicon is an indirect band-gap semiconductor, radiative recombination is strongly suppressed and thus Auger recombination is the dominant intrinsic recombination mechanism over a wide range of dopant concentrations and injection levels, especially for high dopant concentrations or under high injection conditions. Thus, for device simulation and for the interpretation of effective carrier lifetime data, accurate modeling of the Auger recombination as a function of the dopant concentration and the excess carrier density is required.
Auger recombination processes in crystalline silicon are rather complex: Besides the purely collisional processes, where the excess energy is either transferred to an electron (eeh process) or hole (ehh process), the processes can occur with phonon participation or involve impurities [2-4]. Moreover, Auger recombination is influenced by attractive Coulomb interactions of electrons and holes which lead to the formation of excitons. According to the quantum-mechanical theory of Hangleiter and Häcker, this excitation formation leads to an increased density of electrons in the vicinity of holes, which consequently increases the Auger recombination [5].

As the charge carriers involved in the Auger processes are traditionally assumed to be non-interacting quasi-free particles [6-8], the recombination rates of the eeh and the ehh processes are proportional to the involved carrier densities \( R_{eeh} = C_n n^2 p \) and \( R_{ehh} = C_p n^2 p \), where \( C_n \) and \( C_p \) are the Auger coefficients. \( n \) and \( p \) are the electron and hole densities, respectively. To account for the Coulomb-enhanced Auger recombination, \( C_n \) and \( C_p \) are multiplied with enhancement factors \( g_{eeh} \) and \( g_{ehh} \), respectively [5]. Based on experimental lifetime data, Altermatt et al. parameterized the enhancement factors as a function of the dopant concentration and the temperature for n-type and p-type silicon in low-injection condition using an empirical expression [9]. There are only few parameterizations which model the Auger recombination as a function of dopant concentration and the excess carrier density. One of the most widely used parameterization was proposed by Kerr and Cuevas in 2002 [1]. They included the radiative recombination according to Schlangenotto et al. [10] in their parameterization, so that the predicted intrinsic lifetime is given by

\[
\tau_{intr,Kerr} = \frac{\Delta n}{np \left( 1.8 \times 10^{-24} n_0^{0.65} + 6 \times 10^{-25} p_0^{0.65} + 3 \times 10^{-27} \Delta n^{0.8} + 9.5 \times 10^{-15} \right)}
\]  

Over the last 10 years the silicon surface passivation was improved continuously, particularly aluminum oxide (Al₂O₃) resulted in very low surface recombination velocities below 5 cm/s [11-15]. Recently, several authors have reported effective lifetimes exceeding the intrinsic limit of Kerr’s model [12, 16, 17]. This indicates that applying these improved surface passivation layers allow to investigate silicon bulk recombination with an improved precision, and moreover that it is necessary to revise the intrinsic lifetime limit. Meanwhile, also the model of the radiative recombination in silicon [18, 19], as well as lifetime measurement techniques [20-22] were improved. Based on our own lifetime measurements as well as literature lifetime data, we introduce a new parameterization for the intrinsic recombination of p-type and n-type silicon at 300 K, taking the aforementioned recent improvements into account.

2. Auger recombination in silicon solar cells

To illustrate the influence of Auger recombination on silicon solar cells, we performed PC1D simulations [23] exemplarily for an n-type silicon solar cell with front side boron emitter. The simulation was conducted for a 150 μm thick, 1 Ω cm n-type silicon base with a shallow industrial boron doped emitter. Figure 1 shows the recombination current density \( J_{ec,mpp} \) at the maximum power point (mpp), separated into the contributions of the different recombination mechanisms. \( J_{rec,mpp} \) was calculated as a function of the effective rear surface recombination velocity \( S_{eff,rear} \). It can be seen, that with decreasing \( S_{eff,rear} \) the contribution of the Auger recombination increases significantly, reaching about 30% of the total \( J_{rec,mpp} \) at \( S_{eff,rear} = 10 \text{ cm/s} \), while the contribution of the radiative recombination is more than one order of magnitude smaller. By reducing \( S_{eff,rear} \) from 1000 cm/s to 10 cm/s, the minority carrier density in the bulk and in the emitter region is increased by more than one order of magnitude, which consequently
increased the recombination too, in particular for the Auger recombination. This illustrates, that the relevance of the Auger recombination is gaining importance with improving solar cell technology.

3. Lifetime measurement comparison

As a first step, we verified whether our measured effective lifetime data differs significantly from Kerr’s intrinsic lifetime limit by comparing different lifetime measurement techniques at two different laboratories: (i) the photo-conductance decay (PCD) [24-26] measurements at ISFH and (ii) PCD as well as quasi-steady-state photo-luminescence (QSSPL) [27] measurements at Fraunhofer ISE. More details about the measurements can be found in Ref. [28]. This is shown exemplarily for a 1.34 Ω cm p-type FZ Si sample passivated with 10 nm ALD Al2O3. The resulting effective lifetime data is compared in Fig. 2. The upper graph shows the relative deviation of both PCD measurements with respect to the PL measurement. All measurements are in good agreement, particularly in the Auger recombination-dominated injection range above 5×10^14 cm^−3. It is worth mentioning that this agreement is observed for effective lifetime measurement techniques which are based on completely different physical phenomena: the illumination-induced photo-conductance and photo-luminescence. From these lifetime measurement comparison as well as the measurement uncertainties, we estimated a relative uncertainty range of ±20% for our effective lifetime measurements, which is shown in the upper graph of Fig. 2 as dashed gray lines. Fig. 2 also compares the measured lifetime data with τ_{intr,Kerr} according to Eq. (1). The relative deviation with respect to the PL measurement is plotted again in the upper graph. For excess carrier densities Δn > 5×10^14 cm^−3 τ_{intr,Kerr} underestimates the measured effective lifetime considerably,
with a maximum relative deviation of 38%. This deviation is clearly higher than our measurement uncertainty of 20% and thus reveals a significant underestimation.

4. Advanced parameterization of the Auger recombination

We have measured the injection-dependent effective lifetime of high-purity silicon wafers as a function of the dopant concentration of phosphorus-doped n-type and boron-doped p-type silicon wafers which were passivated with Al₂O₃ or SiNₓ. Based on this effective minority carrier lifetime measurements we developed an advanced parameterization of the Auger recombination lifetime as a function of the dopant concentration and the excess carrier density for crystalline silicon at 300 K. We included the radiative recombination according to Refs. [18, 19] which also includes Coulomb-enhanced radiative recombination, thus our parameterization models the complete intrinsic recombination:

$$\tau_{\text{intr,adv}} = \frac{\Delta n}{(np - n_{i,\text{eff}}^2) \left( 2.5 \times 10^{-31} g_{\text{ehh}} n_0 + 8.5 \times 10^{-32} g_{\text{eeh}} p_0 + 3.0 \times 10^{-29} \Delta n^{0.92} + B_{\text{rel},B_{\text{low}}} \right)}$$

(2)

with the enhancement factors:

$$g_{\text{eoh}}(n_0) = 1 + 13 \left( 1 - \tanh \left[ \frac{n_0}{N_{0,eoh}} \right]^{0.66} \right)$$
and
$$g_{\text{ehh}}(p_0) = 1 + 7.5 \left( 1 - \tanh \left[ \frac{p_0}{N_{0,ehh}} \right]^{0.63} \right)$$

(3)

with $N_{0,eoh} = 3.3 \times 10^{17}$ cm⁻³ and $N_{0,ehh} = 7.0 \times 10^{17}$ cm⁻³, and with all other parameters specified in Tab. I. We account separately for the Coulomb-enhanced Auger recombination by applying adapted enhancement factors $g_{\text{eoh}}$ and $g_{\text{ehh}}$ analogously to those introduced by Altermatt et al. [9]. The parameterization provides an excellent accuracy to model the upper limit of the minority carrier lifetime in silicon for the full range of n-type and p-type dopant densities, as well as a broad range of carrier densities.

Table I. Parameters for Eq. (2).

<table>
<thead>
<tr>
<th>param.</th>
<th>unit</th>
<th>Description</th>
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<tr>
<td>$n$</td>
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<td>electron density</td>
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<tr>
<td>$p$</td>
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<td>$p_0$</td>
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<td>cm⁻³</td>
<td>excess carrier density</td>
</tr>
<tr>
<td>$n_i$</td>
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<td>intrinsic carrier concentration for lowly-doped and lowly-injected silicon, 9.7×10¹⁷ cm⁻³ at 300 K [29]</td>
</tr>
<tr>
<td>$n_{i,\text{eff}}$</td>
<td>cm⁻³</td>
<td>effective intrinsic carrier concentration for lowly-doped and lowly-injected silicon, 4.73×10¹⁵ cm⁻³ at 300 K [18]</td>
</tr>
<tr>
<td>$B_{\text{low}}$</td>
<td>cm⁻³ s⁻¹</td>
<td>relative radiative recombination coefficient, according to Ref. [30]</td>
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Fig. 3. Bulk lifetime $\tau_{\text{mb}}$ of an 1.05 $\Omega$ cm p-type FZ Si sample passivated with 30 nm Al₂O₃ using plasma-assisted ALD [28]. The bulk lifetime was determined using the wafer thickness variation method. Also plotted are the modeled intrinsic lifetime $\tau_{\text{mb,Intr}}$ according to Eq. (1) and $\tau_{\text{mb,Adv}}$ according to Eq. (2).
injection levels. In the following, the parameterization is exemplarily discussed for $p$-type silicon. A more detailed discussion can be found elsewhere [28], including reasonable simplifications of the parameterization to improve the practical application, particularly concerning the effective intrinsic carrier concentration and the Coulomb-enhanced radiative recombination, which are both rather complex to calculate.

Fig. 3 compares the bulk lifetime $\tau_{\text{bulk}}$ of an 1.05 $\Omega$ cm $p$-type FZ Si sample with the modeled intrinsic lifetime $\tau_{\text{intr,Kerr}}$ according to Eq. (1) and $\tau_{\text{intr,adv}}$ according to Eq. (2). The bulk lifetime was determined using a wafer thickness variation experiment of mechanically thinned samples [28, 35]. The samples were passivated with 30 nm of Al$_2$O$_3$ using plasma-assisted ALD. The experiment reveals a bulk lifetime as high as 4.5$\pm$0.5 ms at $\Delta n$ around $10^{15}$ cm$^{-3}$ for this 1.05 $\Omega$ cm $p$-type FZ Si [28], which is almost twice the 2.3 ms predicted by $\tau_{\text{intr,Kerr}}$. As can be seen, our advanced parameterization $\tau_{\text{intr,adv}}$ is in excellent agreement with the determined bulk lifetime, in particular in the Auger recombination dominated high injection range.

Fig. 4 shows the maximum measured effective lifetime of our $p$-type samples together with literature data as a function of the dopant concentration. The data is compared to the modeled $\tau_{\text{intr,adv}}$ of Eq. (2), the radiative recombination lifetime according to Trupke et al. [18], and the Coulomb-enhanced radiative recombination lifetime according to Altermatt et al. [30], as well as the free-particle Auger lifetime with Auger coefficients after Dziewior and Schmid [32]. As our prepared lifetime samples cover a dopant concentration range up to $N_{\text{dop}}=2\times10^{17}$ cm$^{-3}$, we used literature data for higher $N_{\text{dop}}$ to fit our parameterization. Thus, for $N_{\text{dop}}>2\times10^{18}$ cm$^{-3}$ $\tau_{\text{intr,adv}}$ is in good agreement with the parameterization of Altermatt et al. [9] and converges to the free particle Auger lifetime. It can also be seen, that for $N_{\text{dop}}<10^{16}$ cm$^{-3}$ the measured effective lifetime is significant below $\tau_{\text{intr,adv}}$. This is typically attributed to extrinsic recombination either from the surface or the bulk [9, 28].

5. Summary

Auger recombination can significantly influence the performance of crystalline silicon based solar cells. This is illustrated by PC1D simulations exemplarily for $n$-type silicon solar cells with varying rear side passivation qualities. Recent advances in surface passivation techniques for silicon wafers based on Al$_2$O$_3$ have allowed to study silicon bulk recombination with an improved precision. By applying Al$_2$O$_3$ passivation layers we found that in some cases the measured effective carrier lifetime exceeds the previously accepted limit for the intrinsic recombination proposed by Kerr and Cuevas [1]. To verify our
measurements we have cross-checked the results with different measurements techniques at two different laboratories. Based on effective lifetime measurements we developed an advanced parameterization of the intrinsic lifetime in crystalline silicon at 300 K which accounts for Coulomb-enhanced Auger recombination and Coulomb-enhanced radiative recombination. This parameterization provides an excellent accuracy for modeling the upper limit of the minority carrier lifetime in crystalline silicon for a wide range of dopant densities, as well as a broad range of carrier injection levels.

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References


