Modelling silicon characterisation

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Abstract

A versatile computer model is presented for the simulation of several characterization techniques commonly used to determine the electronic properties of silicon wafers and solar cells. Several different sets of empirical data for carrier mobility and carrier recombination in crystalline silicon can be optionally selected to investigate their impact on device performance. The model is applicable to arbitrary carrier injection conditions and compensated doping. It is an advanced tool that permits to predict the outcome of characterization experiments, design new ones, or to perform in-depth post-measurement analysis and diagnosis of silicon materials.

Keywords: Modelling, characterisation

1. Introduction

The dissemination of novel characterization techniques has allowed PV engineers to probe silicon wafers for the main electronic properties that define their eventual usefulness to convert sunlight into electricity. These measured properties, in particular the effective carrier lifetime, are not only useful figures of merit, but also an invaluable source of scientific information.

To extract the latter it is necessary to reproduce the experimental conditions with theoretical models that are simple enough to permit physical insight. This paper uses a versatile model [1] (QSSModel, available from http://ssc.cecs.anu.edu.au/) primarily conceived as a scientific tool to simulate photoconductance [2] and luminescence [3] measurements, but capable of determining I-V and spectral response curves as well. To demonstrate its usefulness, we apply the model to a few representative cases and compare it to PC1D [4] in a particularly challenging situation that can occur in silicon solar cells.

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2. Applications of the model

2.1. Effective lifetime vs. excess carrier density

Let us re-examine experimental data for oxide passivated FZ silicon wafers [5] that formed the basis to develop Kerr’s empirical expression for the intrinsic lifetime in silicon [6]. In the modeling, we assume perfect surface passivation and consider the possibility of SRH recombination due to iron contamination. Fig. 1 compares the experimental and modeled carrier lifetime as a function of excess carrier density for three different silicon wafers. The impact of Fe on p-type silicon is so strong that even a very small concentration of \([\text{[Fe]}]=2\times10^{10}\text{cm}^{-3}\) makes the effective lifetime for the 10\(\Omega\text{cm}\) p-type wafer drop significantly at low carrier densities. For the 150\(\Omega\text{cm}\) p-type wafer a good fit to the measured data is obtained for \([\text{[Fe]}]=2.5\times10^{10}\text{cm}^{-3}\), while for the 1.5\(\Omega\text{cm}\) n-type wafer the required iron concentration is slightly higher, \([\text{[Fe]}]=5\times10^{10}\text{cm}^{-3}\). This modeling exercise provides a credible explanation to the puzzling injection dependence of the lifetime at low carrier densities, attributing it to residual Fe contamination.

![Fig. 1. Modelled carrier lifetime as a function of excess carrier density for 150 \(\Omega\text{cm}\) p-type, 10 \(\Omega\text{cm}\) p-type, and 1.5 \(\Omega\text{cm}\) n-type silicon wafers slightly contaminated with iron ([Fe]=2-5x10^{10}\text{cm}^{-3}).](image)

2.2. Device current and voltage at intermediate injection conditions

To demonstrate that the model is applicable to devices in arbitrary injection conditions, we consider an \(n^+pp^+\) solar cell structure with \(N_A=10^{13}\text{cm}^{-3}\), bulk resistivity 1310 \(\Omega\text{cm}\), at short-circuit under AM1.5G illumination. Fig. 2 indicates a very good agreement between QSSModel and PC1D in finding the excess carrier density profile, which presents two peculiar features: a) the carrier density is high at the front junction, implying that this junction is forward biased. b) The carrier density is suppressed in the vicinity of the rear \(pp^+\) junction. Most of the base region remains in high injection, benefiting from “conductivity modulation”, a phenomenon by which excess carriers effectively reduce the resistivity of the material, which makes high resistivity or intrinsic silicon usable for solar cells. Nevertheless, a high electric field develops in the rear part, resulting in a significant electrostatic potential drop of -0.429V. This is perfectly balanced by the voltage at the front junction \(V_{n+p}=0.429\text{V}\), making the total device voltage \(V=0\), as befits short-circuit. The agreement between QSSModel and PC1D in terms of short-circuit current (35.3mA/cm²), open-circuit voltage (~672mV) and efficiency (~19.8%) is also very good.
2.3. Photoluminescence of silicon ingots

The analysis of a photoluminescence measurement involves linking the photon emission to the particular excess carrier density profile occurring in the sample, accounting for self absorption by the silicon [7]. The modeled spectral luminescence in Fig. 3 corresponds to a boron doped, $N_A=10^{16}$ cm$^{-3}$, silicon ingot (no surface passivation) with $[\text{Fe}]=5 \times 10^{12}$ cm$^{-3}$. In this case, the ratio between the integrated PL intensity for the FeB state to that of the Fe$\text{i}$ state is 1.55, similar to the ratio of 1.61 between the carrier diffusion lengths, $102 \mu$m for FeB and $63 \mu$m for Fe$\text{i}$. The assumed illumination wavelength is 810 nm, with an absorption depth of 13 $\mu$m which, together with the high surface recombination, caps the effective lifetime to 15 $\mu$s.

PL modeling can be extended to a Si ingot grown from feedstock containing 0.5 ppmw B, 1.5 ppmw P and 1 ppmw Fe. The actual dopant concentrations in the crystal are in the range $5 \times 10^{16}$ cm$^{-3}$ to $3 \times 10^{17}$ cm$^{-3}$ for B and P and $4 \times 10^{11}$ cm$^{-3}$ to $3 \times 10^{13}$ cm$^{-3}$ for Fe. Fig. 4 shows that the PL intensity has a minimum at approximately the same position where the net dopant density is zero, in agreement with experimental observations by Trupke et al. [8]. The correlation between PL intensity and net doping is modulated by the changes in carrier profile caused by a varying interstitial iron concentration and carrier lifetime.
3. Conclusions

This paper has shown just a few of the many applications that a relatively simple theoretical model can have to better understand the physics that underlie silicon solar cells. The model considers emitter regions as mere surface boundary conditions, it uses simple optics, and a relatively small number of 1D elements in the base region. Nevertheless, the model provides scientists with an advanced tool to predict the outcome of characterization experiments, design new ones, or perform in-depth analysis of measured parameters. It also is a versatile platform where new capabilities can be added by the user.

References


Appendix A. Simplified model of a solar cell in arbitrary injection conditions

The operation of a solar cell can be summarized by the aphorism: *Once generated, carriers that survive recombination exit the solar cell as an electric current*. This can be expressed mathematically as

\[ J = qG_T - qR_T \]  (1)

Determining the output current density \( J \) for an arbitrary device voltage \( V \) requires a detailed analysis of electrons and holes within the device. It is useful to note that the excess carrier density is a proxy for device voltage, which permits to use the former as the input “excitation” in order to find the solution to the problem, that is, \( J \) and \( V \).

For the analysis of p-type base region solar cells, we consider the current positive when flowing towards the right, along the x-axis of our one-dimensional model. Note that a positive electron current is
the consequence of electrons actually moving towards the left. The implementation in the computer program assumes that the n+ region is on the left, so a positive current emerges out of the p-type side of the solar cell, following the common convention.

Even if the device is in open-circuit, there may be internal flows of electrons and holes. If we consider a small volume defined by an interval of distance, $\Delta x$, the concentration of carriers can increase due to the injection of electrons into that volume, $-J_n$, or to the photogeneration occurring within it, $G_L$. The two mechanisms that can make it decrease are the current that leaves the slice of material, $J_n(x+\Delta x)$, and recombination within it, given by $R_v$, the volume recombination rate. In the steady-state these carrier augmentation and reduction mechanisms are perfectly balanced and we can, therefore, write

$$-J_n(x + \Delta x) = -J_n(x) + qG_L(x)\Delta x - qR_v(x)\Delta x$$  

(2)

This equation represents, when the element size is infinitesimally small, the integral form of the continuity equation.

In addition, the transport equations relate the carrier density to the electron current. When a net current $J$ flows, it is composed at any point $x$ of the sum of the electron and hole currents:

$$J_n(x) = J - J_p(x)$$  

(3)

In general, the electron and hole currents are made up of a diffusion term and a drift term. Both can be lumped together into an effective, or ambipolar, diffusion coefficient, $D_{\text{eff}}$:

$$D_{\text{eff}} = \frac{(n + p)D_nD_p}{nD_n + pD_p}$$  

(4)

where $D_n$ and $D_p$ are the diffusion coefficients for electrons and holes. The electron current can thus be expressed as:

$$J_n(x) = qD_{\text{eff}} \frac{dn}{dx} + J \frac{nD_n}{nD_n + pD_p}$$  

(5)

The next step is to integrate over an interval $\Delta x$ small enough so that the electron current can be considered constant within it:

$$\Delta n(x + \Delta x) = \Delta n(x) + J_n(x)\Delta x - \frac{J}{qD_{\text{eff}}} \frac{nD_n}{nD_n + pD_p} \Delta x$$  

(6)

This equation permits to find the electron concentration as a function of position, with the electron current being determined from Eq. 2. Note that $D_{\text{eff}}$ is, in general, injection level dependent and also position dependent. In addition the electron and hole diffusion coefficients, $D_n$ and $D_p$ can be themselves injection level dependent. QSSModel includes several models for electron and hole mobility.

In deriving these equations, valid for any injection level and dopant density, the only assumptions have been that departures from charge neutrality are very small, so that $\Delta n = \Delta p$ (note that this is also necessary for the applicability of the SRH recombination model), and $d\Delta n/dx = d\Delta p/dx$. Both conditions are usually met in silicon solar cells.

The boundary conditions that the carrier density function must satisfy come from the fact that the rate at which carriers flow towards the surface must be equal to the rate at which they recombine there. The latter can be expressed by means of a saturation current density $J_s$. For example, at the front surface:
A similar expression applies to the rear surface. If desired, the minority carrier surface recombination velocity \( \mathcal{S}_n \) can be found from the following definition:

\[
\mathcal{S}_n = \mathcal{S}_p = \frac{R_{\text{surf}}}{\Delta n_{\text{surf}}}
\]  

(8)

In our model the diffused, or emitter, regions have zero thickness and space charge regions have not been included. The full Shockley-Read-Hall bulk recombination model has been implemented, including a look up table with the energy levels and capture cross sections of the most important metal impurities, as well as the B-O complex in CZ silicon. Intrinsic Auger and band to band recombination has been implemented using the empirical expression proposed by Kerr et al. [6].

As a consequence of the different mobilities of electrons and holes, an electric field may develop within the wafer to assist the flow of the latter and help maintain charge neutrality. The consequence of this is an electrostatic potential drop across the base region. This Dember effect voltage is only significant for lowly doped silicon when the carrier profile is very non-uniform. In addition, when a net current \( J \) flows through the base region, it can produce an Ohmic potential drop. To find the total electrostatic potential drop across the base region, \( V_{\text{Base}} \), it is necessary to integrate the electric field. In the following expression the first term represents the “bulk diffusion”, or Dember component and the second term the Ohmic component of the electric field:

\[
\xi = \frac{kT \mu_p - \mu_n}{q} \frac{dn}{dx} + \frac{J}{q (n \mu_n + p \mu_p)}
\]  

(9)

Finally, the terminal voltage of an \( n^+ pp^+ \) solar cell can be found to be:

\[
V_{n^+ pp^+} = \frac{kT}{q} \ln \left( \frac{(n_n + \Delta n_{\text{front}})(p_p + \Delta n_{\text{back}})}{n_i^2} \right) + V_{\text{Base}}
\]  

(10)

The solution corresponding to an n-type base region is formally identical to that of the p-type cell with just one small modification to a term in the carrier density equation (see Eq. 14) and with a change to the sign convention for the current, which is now positive when it flows towards the left. Note that, for both the n-type or p-type cases, a current is positive when flowing out of the p-side terminal. The solution for the excess hole concentration in the n-type quasi-neutral region is:

\[
\Delta p(x + \Delta x) = \Delta p(x) + \frac{J_p(x)}{qD_{\text{eff}}} \Delta x - \frac{J}{qD_{\text{eff}} n \mu_n + p \mu_p} \Delta x
\]  

(14)

When the \( p^+ \) region is at the front, illuminated face, the expression for the terminal voltage of an \( p^+ nn^+ \) solar cell is:

\[
V_{p^+ \text{base} n^+} = \frac{kT}{q} \ln \left( \frac{(p_p + \Delta n_{\text{front}})(n_n + \Delta n_{\text{back}})}{n_i^2} \right) + V_{\text{Base}}
\]  

(15)