Highlights

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Deep neural network method for predicting the iron concentration in silicon solar cell by current-voltage characteristic

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ABSTRACT

Defect-assisted recombination processes frequently limit the photovoltaic device performance. Non–destructive methods of evaluation of the impurities contamination in solar cells, are important from an applied point of view. In this work, we use numerical device simulation to demonstrate the ability to extract impurity contamination from an ideality factor value and utilizing a deep neural network (DNN). The dense layer DNN was trained by using simulation of current-voltage curves of silicon n^+–p–p^+ structure with the following parameters. The iron concentration ranged from 10^{10} to 10^{13} cm^{-3}, the base doping level — from 10^{15} to 10^{17} cm^{-3}, the base thickness — from 150 to 240 micron, and the temperature — from 290 to 340 K. The structure with interstitial iron atoms only as well as with coexistence of Fe_iB_s pairs and Fe_i was under consideration. It is shown that DNN is able to predict iron concentration with mean squared relative error up to 0.03.

1. Introduction

Metal contamination control remains an important challenge for silicon processing both for microelectronics, logic technologies and solar cells (SCs) [1, 2, 3, 4]. Typically, metal related defect characterization is performed by Fourier-transform infrared spectroscopy, electron-paramagnetic resonance, minority carrier lifetime measurements, deep level transient spectroscopy (DLTS), Laplace DLTS etc [5, 6, 7]. However, these techniques are time-consuming, require special equipment or/and sample preparing. At the same time, the current-voltage (IV) measurement is a standard rapid industrial SC characterization technique. IV characteristics contain important information about electrically active defects [6, 8]. And a few defect diagnostics by IV characteristics are proposed [6, 8, 9, 10, 11]. The temperature dependencies of current components [10, 11] or IV differential parameters [8, 9] are under consideration. But the numerous and high accuracy IV measurements are required in the first and second cases, respectively.

In our previous work [12], we have shown that the SC ideality factor value (n) can be used to estimate the iron concentration (N_{Fe}). It should be noted that the ideality factor is quite often used to characterize the various semiconductor barrier structures [13, 14, 15, 16, 17]. However, a defect's signature in an ideality factor is convoluted with those from so many other physical processes. As a result the obtained analytic expressions $N_{Fe} = f(n)$ are not general and the numerous grading curves are needed to N_{Fe} determination [12]. On the other hand, in the last decade, the deep learning, which is enable to solve problems without clear algorithmization, have been successfully used in various fields of theoretical and applied physics [18, 19, 20]. Furthermore, materials informatics (combination of material property calculations/measurements and informatics algorithms) has been asserted [21] to become the fourth (along with theory, simulations, and experiments) paradigm of science. The aim of this work is to apply the deep learning approach for predicting the iron concentration from ideality factor (so to say "deep learning for deep levels"). Further, unlike in previous work [12], the back surface field (BSF) n^+–p–p^+ structure was under consideration and the base thickness influence on ideality factor was taken into account as well.

As the approximation to the practical using, the paper considers a fairly simple system which consists of crystalline silicon (c-Si) SC and iron impurity. However, the system is important in practice. Silicon solar cells constitute 90% of current global production capacity [22] and BSF is one of popular designs used for industrial mass production of c-Si SCs [23]. Iron is a major as one of the most detrimental metal impurities in c-Si SCs [2, 3, 4]. The flowchart of the used heuristic approach is shown in Fig. 1. The following milestones can be distinguished. First, the dark IV characteristic is simulated for SCs with both known contaminant composition and various parameters. In our numerical simulation

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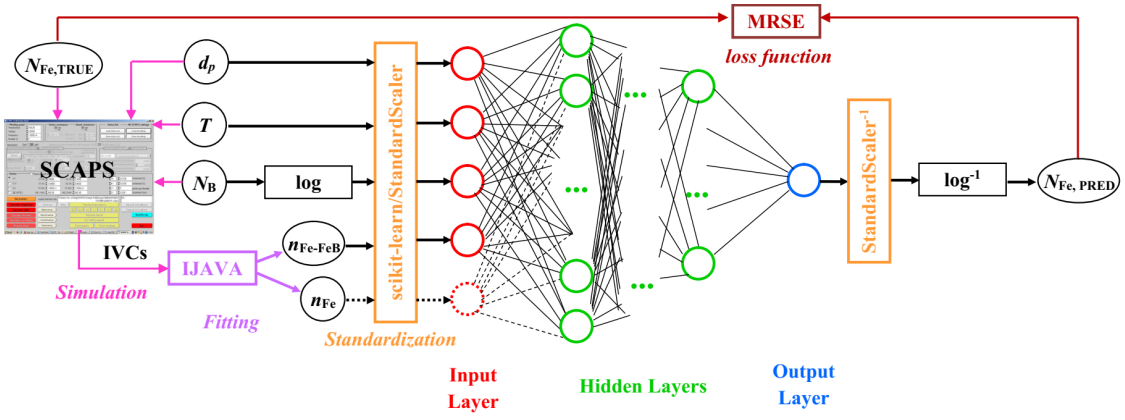

Figure 1: Schematic of deep learning based approach for predicting the iron concentration. Additional details are discussed in the body of the article.

we make use of SCAPS-1D [24, 25], which widely used to model silicon-based devices [26, 27, 28]. Second, the obtained characteristic is fitted according to the double-diode model and the ideality factor is estimated. As a result of aforesaid steps, the labeled datasets were produced. Obviously, the labeled dataset from experimental IVs would be preferable, but it is practically difficult to find the thousands of samples with the required parameters. Third, the training of deep neural network (DNN) to estimate an iron contamination by using SC's base thickness, doping level, temperature, and ideality factor value. Fours, the DNN testing.

2. Simulation Details

The presented calculation uses n^+–p–p^+ structure. n^+ is the emitter layer with the donor concentration $N_D = 10^{19}$ cm^{-3} and the thickness 0.5 μm. p and p^+ are the base and BSF-layer, respectively, which are uniformly doped with boron. 1 μm and 5×10^{18} cm^{-3} are the thickness d_{BSF} and the acceptor concentration N_{BSF} of the p^+ layer. The base with the thickness $d_p = 150$–240 μm is doped with concentration $N_B = 10^{15}$–10^{17} cm^{-3}.

The simulations were carried out over the temperature range $290 - 340$ K. The SCAPS setting file was created for each temperature using the following material parameters. The bandgap E_G and bandgap narrowing ΔE_G models are, respectively, from Pässler [29] and Yan and Cuevas [30]:

$$E_G = E_{G0} - \alpha\Theta\left\{\frac{1-3\Delta^2}{e^{\frac{\Theta}{T}}-1} + \frac{3\Delta^2}{2}\left(\sqrt[6]{1+\frac{\pi^2}{3(1+\Delta^2)}\left(\frac{2T}{\Theta}\right)^2 + \frac{3\Delta^2-1}{4}\left(\frac{2T}{\Theta}\right)^3 + \frac{8}{3}\left(\frac{2T}{\Theta}\right)^4 + \left(\frac{2T}{\Theta}\right)^6} - 1\right)\right\}, \quad (1)$$

$$\Delta E_G = 4.20\times10^{-5}\left[\ln\left(\frac{N_D}{10^{14}}\right)\right]^3; \qquad \Delta E_G = 4.72\times10^{-5}\left[\ln\left(\frac{N_{B,BSF}}{10^{14}}\right)\right]^3, \quad (2)$$

where $E_{G0} = 1.1701$ eV, $\alpha = 3.23 \times 10^{-4}$ eV/K, $\Theta = 446$ K, $\Delta = 0.51$. The carrier thermal velocities are calculated from models by Green [31]:

$$\upsilon_{\mathrm{th},n} = \sqrt{\frac{8qkT}{0.28m_0\pi}}; \qquad \upsilon_{\mathrm{th},p} = \sqrt{\frac{8qkT}{0.41m_0\pi}}, \quad (3)$$

where m_0 is the free electron mass. The effective states density masses in the conduction band m^*_{dC} and the valence band m^*_{dV} are calculated according to models from Couderc et al. [32]:

$$\left(\frac{m^*_{dC}}{m_0}\right)^{1.5} = 1.094 - 1.312\times10^{-5}T + 6.753\times10^{-7}T^2 + 4.609\times10^{-10}T^3, \quad (4)$$

$$\left(\frac{m^*_{dV}}{m_0}\right)^{1.5} = 0.3426 + 3.376\times10^{-3}T - 4.689\times10^{-6}T^2 + 2.525\times10^{-9}T^3\,. \quad (5)$$

The carrier mobilities and the free carrier effective masses are from Klaassen [33] and O'Mara et al. [34], respectively. The temperature and doping dependencies of Auger recombination coefficients are calculated from models by Altermatt et al. [35]:

$$C_p(T) = (7.91\times10^{-32} - 4.13\times10^{-35}T + 3.59\times10^{-37}T^2) \times\left(1 + \left(564812T^{-1.6545} - 1\right)\left(1 - \tanh\left[\left\{\frac{p}{5\times10^{16}}\right\}^{0.29}\right]\right)\right), \quad (6)$$

$$C_n(T) = 2.8\times10^{-31}\times\left(1 + \left(235548T^{-1.5013} - 1\right)\left(1 - \tanh\left[\left\{\frac{n}{5\times10^{16}}\right\}^{0.34}\right]\right)\right). \quad (7)$$

The Auger recombination coefficient is from Nguyen et al. [36].

The outside surface recombination with electron and hole velocities 10^3 cm/s was taken into account.

The simulations are carried out under the assumption that the defect–assisted recombination is connected with iron–related deep levels only. As the base and the SBF-layer uniform contaminant, iron is assumed to be in concentration $N_{\rm Fe} = 10^{10}$–10^{13} cm^{-3}. The simulations have been performed for the following two cases. In the first one, the concentration of totally dissolved iron is given by a sum of the concentration of the interstitial iron Fe_i and the concentration of trigonal iron-boron pair Fe_iB_s:

$$N_{\rm Fe} = N_{{\rm Fe}_i} + N_{{\rm Fe}_i{\rm B}_s}\,. \quad (8)$$

The defect distributions are uniform, depend on the Fermi level F position, and are given by [37, 38]:

$$\frac{N_{\rm FeB}}{N_{\rm Fe}} = \frac{N_{\rm B}10^{-23}\exp\left(-\frac{E_b}{kT}\right)}{\left[1 + \frac{N_{\rm B}}{10^{23}}\exp\left(-\frac{E_b}{kT}\right)\right]\left[1 + \exp\left(-\frac{F - E_{{\rm Fe}_i}}{kT}\right)\right]}, \quad N_{{\rm Fe}_i} = N_{\rm Fe} - N_{\rm FeB}\,, \quad (9)$$

where $E_b = 0.582$ eV is the binding energy of the Fe_iB_s pairs, $E_{{\rm Fe}_i}$ is the donor level, associated with Fe_i. This case correspond to the equilibrium condition and is labeled "Fe-FeB" from now on.

In the second one, the Fe_i is suggested to be only present with uniform distribution ($N_{{\rm Fe}_i} = N_{\rm Fe}$). This case can be realized by heat treatment (210°C, 3 min) [39] or intense illumination [40] and is referred as "Fe-FeB" hereafter.

The donor level $E_{{\rm Fe}_i} = E_V + 0.394$ eV with electron $\sigma_{n,{\rm Fe}} = 3.47\times10^{-11}T^{-1.48}$ cm^2 and hole $\sigma_{p,{\rm Fe}} = 4.54\times10^{-16}\exp\left(-\frac{0.05}{kT}\right)$ cm^2 capture cross-sections [37, 41] is associated with Fe_i in simulations. The donor level $E^{\rm D}_{\rm FeB} = E_V + 0.10$ eV, $\sigma^{\rm D}_{n,{\rm FeB}} = 4\times10^{-13}$ cm^2, $\sigma^{\rm D}_{p,{\rm FeB}} = 2\times10^{-14}$ cm^2 and acceptor level $E^{\rm A}_{\rm FeB} = E_C - 0.26$ eV, $\sigma^{\rm A}_{n,{\rm FeB}} = 5.1\times10^{-9}T^{-2.5}$ cm^2, $\sigma^{\rm A}_{p,{\rm FeB}} = 3.32\times10^{-10}\exp\left(-\frac{0.262}{kT}\right)$ cm^2 [42, 37, 41] are used for Fe_iB_s.

The dark forward IV characteristic were generated by SCAPS over a voltage range up to 0.45 V. According to the two-diode model, the dark SC current is given by [43]

$$I = I_{01}\left[\exp\left(-\frac{q(V - R_sI)}{kT}\right) - 1\right] + I_{02}\left[\exp\left(-\frac{q(V - R_sI)}{nkT}\right) - 1\right] + \frac{V - R_sI}{R_{sh}}\,, \quad (10)$$

where I_{01} and I_{02} are the saturation currents, R_{sh} and R_s are the shunt and series resistances. The two-diode model are often used to describe real Si SCs and we used Eq. 10 to fit the simulated data by taking n, I_{01}, I_{02}, R_{sh}, and R_s as fitting parameters. The fitting was performed by using the meta–heuristic method IJAVA [44]. It should be noted that influence of both R_s (obtained values $< 10^{-2}$ Ω) and R_{sh} (obtained values $> 10^{18}$ Ω) can be neglected in simulated IV.

It is the ideality factor value n which is used in our further calculation. The ideality factors, which are obtained in Fe-case and Fe-FeB-case, are referred as $n_{\rm Fe}$ and $n_{\rm Fe-FeB}$ hereafter. The typical simulated dependencies of the ideality factor are shown in Fig. 2. The detailed discussion about $n_{\rm Fe}$ and $n_{\rm Fe-FeB}$ values are presented elsewhere [45], however it should be noted that (i) n can takes equal values for different SC parameters values; (ii) dependencies of $n_{\rm Fe}$ and $n_{\rm Fe-FeB}$ varies slightly.

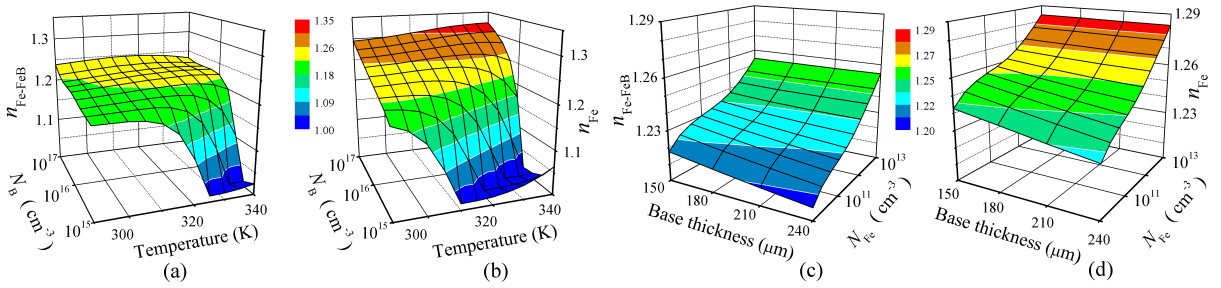

Figure 2: Ideality factor versus temperature and boron concentration (a, b) or base thickness and iron concentration (c,d). The Fe-FeB-case (a, c) and Fe-case (b, d). $N_{\mathrm{Fe}} = 10^{10}$ cm^{-3} (a,b), $d_p = 180$ μm (a, b), $N_{\mathrm{B}} = 10^{16}$ cm^{-3} (c, d), $T = 320$ K (c, d).

3. Deep neural network

Training a deep neural network requires a large number of samples. In order to build a training dataset, we used IV characteristics, which are simulated by using 4 d_p values, 9 N_{B} values, 11 T values and 19 N_{Fe} values. These base thickness, doping level, temperature, and iron concentration values are regularly (for T and d_p in linear scale, for N_{Fe} and N_{B} in logarithmic scale) distributed over the ranges 150–240 μm, 10^{15}–10^{17} cm^{-3}, 290 – 340 K, and 10^{10}–10^{13} cm^{-3}, respectively. Thus, 7524 IV characteristics are simulated in Fe-case as well as in Fe-FeB-case to to build a training dataset.

Besides, several test datasets are prepared. The d_p, N_{B}, and N_{Fe} values, which equal to values from training dataset and T values, which is divergent from training dataset are used to build the test dataset, labeled "T-varied". These dataset is based on 894 pairs of IV characteristics. The similar approach was used to prepare "d-varied" (1189 samples), "Fe-varied" (856 samples), and "B-varied" (514 samples) test datasets. The base thickness, doping level, temperature, and iron concentration values, which are divergent from training dataset values, are used to prepare "All-varied" (684 samples).

The precise parameters values are listed in Supplementary Material.

We have tried to construct the DNN, which is able to estimate iron contamination by using SC parameters (d_p and N_{B}), IV measurement temperature, and result of IV fitting (ideality factor value). As it is shown in Fig. 1 two DNNs with different input parameters were under consideration. The input sample of the first one consist of $\{d_p, N_{\mathrm{B}}, T, n_{\mathrm{Fe-FeB}}\}$. In practice, these input set can be obtained from one dark IV measurement. These neural network referred as $\mathrm{DNN}_{\mathrm{FeFeB}}$ hereafter. The second one uses $\{d_p, N_{\mathrm{B}}, T, n_{\mathrm{Fe-FeB}}, n_{\mathrm{Fe}}\}$ in input layer. In practice, the obtaining of such a set requires additional SC processing (e.g. intense illumination) and two IV measuring. The label $\mathrm{DNN}_{\mathrm{FeFeB-Fe}}$ is used below.

4. Results and discussion

As a result of aforesaid steps, the labeled datasets were produced.

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3. fleqn.clo for left aligned equations;
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The `table` environment is handy for marking up tabular material. If users want to use multirow.sty, array.sty, etc., to fine control/enhance the tables, they are welcome to load any package of their choice and cas-sc.cls will work in combination with all loaded packages.

Table 1
This is a test caption. This is a test caption. This is a test caption. This is a test caption.

Col 1	Col 2	Col 3	Col4
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9. Theorem and theorem like environments

cas-sc.cls provides a few shortcuts to format theorems and theorem-like environments with ease. In all commands the options that are used with the `\newtheorem` command will work exactly in the same manner. cas-sc.cls provides three commands to format theorem or theorem-like environments:

```
\newtheorem{theorem}{Theorem}
\newtheorem{lemma}[theorem]{Lemma}
\newdefinition{rmk}{Remark}
\newproof{pf}{Proof}
\newproof{pot}{Proof of Theorem \ref{thm2}}
```

The `\newtheorem` command formats a theorem in LaTeX's default style with italicized font, bold font for theorem heading and theorem number at the right hand side of the theorem heading. It also optionally accepts an argument which will be printed as an extra heading in parentheses.

```
\begin{theorem}
 For system (8), consensus can be achieved with
 $\|T_{\omega z}$ ...
   \begin{eqnarray}\label{10}
   ....
   \end{eqnarray}
\end{theorem}
```

Theorem 1. *For system (8), consensus can be achieved with* $\|T_{\omega z}$ ...

$$....\tag{11}$$

The `\newdefinition` command is the same in all respects as its `\newtheorem` counterpart except that the font shape is roman instead of italic. Both `\newdefinition` and `\newtheorem` commands automatically define counters for the environments defined.

The `\newproof` command defines proof environments with upright font shape. No counters are defined.

10. Enumerated and Itemized Lists

cas-sc.cls provides an extended list processing macros which makes the usage a bit more user friendly than the default LaTeX list macros. With an optional argument to the `\begin{enumerate}` command, you can change the list counter type and its attributes.

```
\begin{enumerate}[1.]
\item The enumerate environment starts with an optional
  argument ‘1.’, so that the item counter will be suffixed
  by a period.
\item You can use ‘a)’ for alphabetical counter and ’(i)’ for
  roman counter.
 \begin{enumerate}[a)]
   \item Another level of list with alphabetical counter.
   \item One more item before we start another.
   \item One more item before we start another.
   \item One more item before we start another.
   \item One more item before we start another.
```

Further, the enhanced list environment allows one to prefix a string like ‘step’ to all the item numbers.

```
\begin{enumerate}[Step 1.]
 \item This is the first step of the example list.
 \item Obviously this is the second step.
 \item The final step to wind up this example.
\end{enumerate}
```

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`thebibliography` environment. Each reference is a `\bibitem` and each `\bibitem` is identified by a label, by which it can be cited in the text:

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- Parenthetical: `\citep{WB96}` produces (Wettig & Brown, 1996).
- Textual: `\citet{ESG96}` produces Elson et al. (1996).
- An affix and part of a reference: `\citep[e.g.][Ch. 2]{Gea97}` produces (e.g. Governato et al., 1997, Ch. 2).

In the numbered scheme of citation, `\cite{<label>}` is used, since `\citep` or `\citet` has no relevance in the numbered scheme. natbib package is loaded by cas-sc with `numbers` as default option. You can change this to author-year or harvard scheme by adding option `authoryear` in the class loading command. If you want to use more options of the natbib package, you can do so with the `\biboptions` command. For details of various options of the natbib package, please take a look at the natbib documentation, which is part of any standard LaTeX installation.

A. My Appendix

Appendix sections are coded under `\appendix`.

`\printcredits` command is used after appendix sections to list author credit taxonomy contribution roles tagged using `\credit` in frontmatter.

CRediT authorship contribution statement

Oleg Olikh: Conceptualization, Methodology, Formal analysis, Data Curation, Writing - Review & Editing, Visualization, Supervision. **Oleg Lozitsky:** Software, Validation, Investigation, Writing - Original Draft. **Oleksii Zavhorodnii:** Software, Validation, Formal analysis, Writing - Original Draft.

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