

Estimation for iron contamination in Si solar cell by ideality factor: deep neural network approach

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Defect-assisted recombination processes frequently limit the photovoltaic device performance. The low-cost and express methods of impurity contamination control are in demand at solar cell manufacturing. In this paper, we applied deep learning-based approach to extract the iron concentration in silicon solar cells from an ideality factor values. SCAPS-1D was the software of choice for the simulation of solar cells with the back surface field design and for the generation of labeled training and test datasets. Our results demonstrated the deep neural network ability to predict iron concentration by using ideality factor values, temperature, and base thickness as well as doping level of a solar cell. The simulation shows that the prediction error is reduced for high doping level, low temperature, and using of two values of ideality factor (for structure with interstitial iron atoms only as well as for structure with coexistence of Fe_i and iron-boron pair). The capability of functioning of the proposed method is verified for real silicon structures.

KEYWORDS

ideality factor, silicon, $n^+ - p - p^+$ structure, iron contamination, SCAPS, machine learning

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 preparation. At the same time, the current-voltage (IV) measurements are the standard rapid industrial SC characterization technique. IV characteristics contain important information about electrically active defects [6, 8]. And several methods are proposed for diagnosing defects using the IV characteristic [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, obtained analytic expressions $N_{Fe} = f(n)$ are not general and the numerous grading curves are required to determine N_{Fe} ; besides the IV measurements over a temperature range are necessary [12]. On the other hand, in the last decade, deep learning, which enables solving problems without clear algorithmization, has 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. This work aims to apply the deep learning approach for predicting the iron concentration from the ideality factor value (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 influence of the base thickness on ideality factor was taken into account as well.

As the approximation to the practical using, the paper considers a fairly simple system that 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 the popular designs used for industrial mass production of c-Si SCs as yet [23, 24]. Surely, the passivated emitter and rear cell technology has recently come to the fore, but PERC solar cells contain $n^+ - p$ junction as well [24, 25]. Iron is a major as well as one of the most detrimental metallic impurities in c-Si SCs [2, 3, 4]. The flowchart of the used heuristic approach is shown in Fig. 1. The following constituents can be marked out. First, the dark IV characteristics are simulated for SCs with known contaminant composition and various parameters. In our numerical simulation we applied SCAPS-1D [26, 27], which widely used to model solar cells [28, 29, 30, 31, 32, 33]. Second, the obtained IV curves are fitted according to the double-diode model and the ideality factors are estimated. As a result of the 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 iron contamination by using SC's base thickness, doping level, temperature, and ideality factor value. Fours, the DNN testing by using synthetic IV curves as well as experimental IV curves.

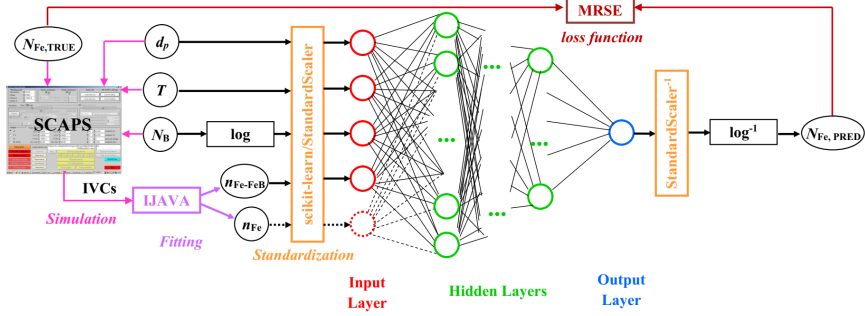


FIGURE 1 Schematic of deep learning-based approach for predicting the iron concentration. Additional details are discussed in the body of the article.

2 | SIMULATION DETAILS

The presented calculation uses $n^+ - p - p^+$ structure: the emitter layer n^+ with the donor concentration $N_D = 10^{19} \text{ cm}^{-3}$ and the thickness $0.5 \mu\text{m}$; p and p^+ are uniformly doped with boron; the base p with the thickness $d_p = 150\text{--}240 \mu\text{m}$ is doped with concentration $N_B = 10^{15}\text{--}10^{17} \text{ cm}^{-3}$ and the BSF-layer p^+ with the thickness d_{BSF} ($1 \mu\text{m}$) and the acceptor concentration N_{BSF} ($5 \times 10^{18} \text{ cm}^{-3}$).

The simulations were carried out over the temperature range $290\text{--}340 \text{ K}$. 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 [34] and Yan and Cuevas [35]:

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

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

where $E_{G0} = 1.1701 \text{ eV}$, $\alpha = 3.23 \times 10^{-4} \text{ eV/K}$, $\Theta = 446 \text{ K}$, $\Delta = 0.51$. The carrier thermal velocities are calculated from models by Green [36]:

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

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. [37]:

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

$$\left(\frac{m_{dV}^*}{m_0} \right)^{1.5} = 0.3426 + 3.376 \times 10^{-3}T - 4.689 \times 10^{-6}T^2 + 2.525 \times 10^{-9}T^3. \quad (5)$$

The carrier mobilities and the free carrier effective masses were taken from Klaassen [38] and O'Mara et al. [39], respectively. The temperature and doping dependencies of Auger recombination coefficients are calculated from

models by Altermatt et al. [40]:

$$C_p(T) = (7.91 \times 10^{-32} - 4.13 \times 10^{-35} T + 3.59 \times 10^{-37} T^2) \times \left(1 + (564812 T^{-1.6545} - 1) \left(1 - \tanh \left[\left\{ \frac{p}{5 \times 10^{16}} \right\}^{0.29} \right] \right) \right), \quad (6)$$

$$C_n(T) = 2.8 \times 10^{-31} \times \left(1 + (235548 T^{-1.5013} - 1) \left(1 - \tanh \left[\left\{ \frac{n}{5 \times 10^{16}} \right\}^{0.34} \right] \right) \right). \quad (7)$$

The band-to-band radiation recombination coefficient was taken from Nguyen et al. [41].

The outside surface recombination with electron and hole velocities 10^3 cm/s was taken into account. The flat bands conditions were assumed for metal contacts on the rear and front surfaces.

The simulations are carried out under the assumption that the defect-assisted recombination corresponds to the iron-related deep levels only. As the base and the SBF-layer uniform contaminant, iron is assumed to be in concentration $N_{Fe} = 10^{10} - 10^{13} \text{ cm}^{-3}$. It is known that Fe in silicon can be in two states: in the form of FeB pair or in the interstitial state Fe_i . At near room temperature and boron concentration $> 10^{14} \text{ cm}^{-3}$, almost all Fe bound in FeB pairs is in equilibrium [42, 43, 44, 45]. According to Wijaranakula[42], the concentration of interstitial iron atoms N_{Fe_i} which remain unpaired in equilibrium state depend on temperature, doping level, and Fermi level F position. The estimations show that at 340 K $N_{Fe_i} \approx 0.1 N_{Fe}$ for $N_B \approx 10^{15} \text{ cm}^{-3}$ in the quasi-neutral region of SC base. However, numerous researches show that temporarily dissociation of pairs can be performed either by heating to the temperature above 200°C , or by intense illumination at room temperature [43, 45].

The simulations have been performed for the following two cases. In the first one, the concentration of total dissolved iron is given by a sum of concentrations of the interstitial iron Fe_i and the trigonal iron-boron pair Fe_iB_s :

$$N_{Fe} = N_{Fe_i} + N_{Fe_iB_s}. \quad (8)$$

The defect distributions in base and p^+ -layer are inhomogeneous, and depend on the Fermi level F position, and are given by [46, 42]:

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

where $E_b = 0.582 \text{ eV}$ is the binding energy of the Fe_iB_s pairs, E_{Fe_i} is the donor level, associated with Fe_i . This case corresponds to the equilibrium condition and in this article will be referred to as “Fe-FeB”.

In the second one, the Fe_i is suggested to be presented only with homogeneous distribution ($N_{Fe_i} = N_{Fe}$). This case can be realized by heat treatment (210°C , 3 min) [47] or intense illumination [48] and will be referred as “Fe” hereafter.

The donor level $E_{Fe_i} = E_V + 0.394 \text{ eV}$ with electron $\sigma_{n,Fe} = 3.47 \times 10^{-11} T^{-1.48} \text{ cm}^2$ and hole $\sigma_{p,Fe} = 4.54 \times 10^{-16} \exp\left(-\frac{0.05}{kT}\right) \text{ cm}^2$ capture cross-sections [46, 49] is associated with Fe_i in simulations. The donor level $E_{FeB}^D = E_V + 0.10 \text{ eV}$, $\sigma_{n,FeB}^D = 4 \times 10^{-13} \text{ cm}^2$, $\sigma_{p,FeB}^D = 2 \times 10^{-14} \text{ cm}^2$ and acceptor level $E_{FeB}^A = E_C - 0.26 \text{ eV}$, $\sigma_{n,FeB}^A = 5.1 \times 10^{-9} T^{-2.5} \text{ cm}^2$, $\sigma_{p,FeB}^A = 3.32 \times 10^{-10} \exp\left(-\frac{0.262}{kT}\right) \text{ cm}^2$ [50, 46, 49] are used for Fe_iB_s .

The dark forward IV characteristics 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 [51]

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

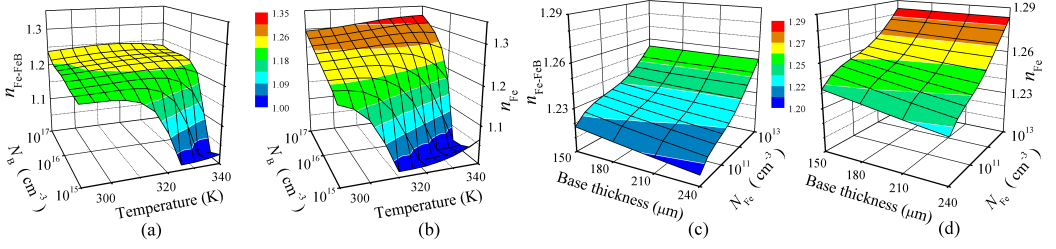


FIGURE 2 Ideality factor versus temperature and boron concentration (a, b) or base thickness and iron concentration (c, d). The Fe-FeB-case (a, c) and Fe-case (b, d). $N_{Fe} = 10^{10} \text{ cm}^{-3}$ (a, b), $d_p = 180 \mu\text{m}$ (a, b), $N_B = 10^{16} \text{ cm}^{-3}$ (c, d), $T = 320 \text{ K}$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

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 is often applied for description of real Si SCs and the first diode represents the “ideal” diode and first term in Eq. (10) current is due to recombination in the base and the emitter, including their surfaces; the second diode is the so-called recombination diode and second term is due to recombination within the depletion region [51]. 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 [52]. The typical example of IV curves and fitting results is shown in Supplementary Material. It should be noted that i) the influence of both R_s (obtained values $< 10^{-2} \Omega$) and R_{sh} (obtained values $> 10^{18} \Omega$) can be neglected in simulated IV; ii) the contribution of recombination diode current is essential at low bias only and the voltage range (0 – 0.45) V is quite sufficient for an accurate determination of the ideality factor values.

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 to as n_{Fe} and n_{Fe-FeB} hereafter. The typical simulated dependencies of the ideality factor are shown in Fig. 2. The detailed discussion about n_{Fe} and n_{Fe-FeB} values are presented elsewhere [53], however it should be noted that (i) n can take equal values for different values of SC parameters; (ii) dependencies of n_{Fe} and n_{Fe-FeB} vary not only in absolute values but although in behavior slightly.

3 | DEEP NEURAL NETWORK MODELS

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 with using of 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 build a training dataset.

Besides, several test datasets are prepared. For instance, the test dataset, labeled “Fe-varied” consist of two subset. The N_{Fe} values 1.300×10^{10} , 2.471×10^{10} , 4.696×10^{10} , 8.927×10^{10} , 1.697×10^{11} , 3.225×10^{11} , 6.130×10^{11} , 1.165×10^{120} , 2.214×10^{12} , 4.209×10^{12} , $8.000 \times 10^{12} \text{ cm}^{-3}$ (which does not used during training data set creation), T values 290, 295, 300, 305, 310, 315, 320, 325, 330, 335, 340 K (which used during training data set creation), d_p value 180 μm (which used during training data set creation), and N_B values 1.778×10^{15} , 5.623×10^{15} , 10^{16} , 3.162×10^{16} , 10^{17} cm^{-3} (which used during training data set creation) were used to prepare the first subset. Thus the first subset is base on 605 pairs of IV characteristics. The N_{Fe} values 1.200×10^{10} , 2.234×10^{11} , 4.160×10^{11} , 7.746×10^{11} , 1.442×10^{12} , 2.685×10^{12} , $5.000 \times 10^{12} \text{ cm}^{-3}$ (which does not used during training data set creation), T values 290, 300, 310, 320, 330, 340 K

(which used during training data set creation), d_p values 210, 240 μm (which used during training data set creation), and N_B values 3.162×10^{15} , 10^{16} , 10^{17} cm^{-3} (which used during training data set creation) were used to prepare the second subset of Fe-varied test dataset. Thus Fe-varied test dataset is based on $605 + 252 = 857$ pairs of IV characteristics.

The similar approach was used to prepare “d-varied” (1189 samples), “T-varied” (832 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 values of parameters are listed in Supplementary Material.

We have tried to construct the DNN, which can estimate iron contamination by using SC parameters (d_p and N_B), measurement temperature, and the 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 $\{d_p, \log N_B, T, \eta_{\text{Fe-FeB}}\}$. In practice, this input set can be obtained from one dark IV measurement. This neural network is referred to as $\text{DNN}_{\text{FeFeB}}$ hereafter. The second one uses $\{d_p, \log N_B, T, \eta_{\text{Fe-FeB}}, \eta_{\text{Fe}}\}$ in input layer. In practice, the obtaining of such a set requires additional SC processing (e.g., intense illumination) and two IV measurements. The label $\text{DNN}_{\text{FeFeB-Fe}}$ is used below.

The dense deep neural network was implemented through the high-level Keras API provided by TensorFlow [54]. The input layers consist of 4 or 5 nodes — see Fig. 1. 1 node and linear activation were used in the output layer. The five configurations of hidden layers were under consideration: (i) “pipe”: each hidden layer contains equal number of nodes; (ii) “trapezium”: six hidden layers, number of neurons linearly decreases from 100% (first layer) to 50% (last layer); (iii) “triangle”: ten layers, number of neurons linearly decreases from 100% (first layer) to 10% (last layer); (iv) “butterfly”: two serial reflected trapezium configurations; (v) “fir”: two serial trapezium configurations.

The mean squared relative error (MSRE) was chosen as the loss function:

$$\text{MSRE} = \frac{1}{N_s} \sum_{i=1}^{N_s} \frac{(N_{\text{Fe,TRUE},i} - N_{\text{Fe,PRED},i})^2}{N_{\text{Fe,TRUE},i} \cdot N_{\text{Fe,PRED},i}}, \quad (11)$$

where N_s is the number of samples in dataset, $N_{\text{Fe,TRUE},i}$ is the iron concentration, which was used in simulation of i -th sample, $N_{\text{Fe,PRED},i}$ is the DNN prediction for i -th sample.

Hyperparameters include the number of nodes for the first hidden layer, the number of hidden layers (in pipe configuration), the batch size, the activation function, the optimizer, the learning rate, the preprocessing method, the dropout rate, the regularization function, the regularization rate, and the weight initializer. A grid search (coarse tuning to limit one hyperparameter) and random search (fine tuning) were performed over the predefined hyperparameter space, shown in Table 1, and the best hyperparameter combination is chosen.

10-fold cross-validation was used to estimate DNN training. The MSRE, coefficient of determination R^2 , and coefficient of correlation R were three metrics used to evaluate the performance of the DNN models on test datasets. Finally, to increase a DNNs performance, the full dataset, which consists of training dataset and all test datasets, was used for the training models.

4 | RESULTS AND DISCUSSION

4.1 | Synthetic IV curves

The results of the hyperparameter search are listed in Table 2. In particular, the trapezium and pipe configurations are chosen for $\text{DNN}_{\text{FeFeB}}$ and $\text{DNN}_{\text{FeFeB-Fe}}$ respectively.

The training and test results of $\text{DNN}_{\text{FeFeB}}$ are presented in Table 3, Table 4, and Fig. 3. As we can see, that MSRE of

TABLE 1 Hyperparameter space for DNNs.

Hyperparameter	Values
# nodes for first hidden layer	30, 40, 50, 75, 100, 120, 150
# hidden layers	4, 5, 6, 8, 10, 15
batch size	8, 16, 32, 64, 128
activation function	ReLu, sigmoid, tanh, SELU, ELU
optimizer	SGD, RMSprop, Adam, Adadelata, Adagrad, Adamax, Nadam, Ftrl
learning rate	10^{-5} , 10^{-4} , 10^{-3} , 10^{-2}
# epochs	100, 300, 400, 600, 1000, 1500
preprocessing method	StandartScaler, MinMaxScaler
regularization function	None, L2, L1, Dropout
regularization rate	10^{-5} , 10^{-4} , 10^{-3} , 10^{-2}
dropout rate	0.2, 0.3, 0.4, 0.5
weight initializer	Xavier Normal or Uniform, He Normal or Uniform, Random Normal or Uniform, Ones

TABLE 2 Chosen hyperparameter combinations.

Hyperparameter	DNN _{FeFeB}	DNN _{FeFeB-Fe}
# nodes for hidden layers	120, 108, 96, 84, 72, 60	100, 100, 100, 100
batch size	32	32
activation function	ReLu	ELU
optimizer	Adamax	Adamax
learning rate	10^{-3}	10^{-3}
# epochs	400	1500
preprocessing method	StandartScaler	StandartScaler
regularization function	None	None
weight initializer	Xavier Normal	Xavier Normal

TABLE 3 Results of 10-fold cross-validation

Dataset	MSRE	
	$\text{DNN}_{\text{FeFeB}}$	$\text{DNN}_{\text{FeFeB-Fe}}$
training	0.31 ± 0.07	0.03 ± 0.01
full	0.28 ± 0.05	0.03 ± 0.01

TABLE 4 DNN's testing results

Dataset	$\text{DNN}_{\text{FeFeB}}$			$\text{DNN}_{\text{FeFeB-Fe}}$		
	MSRE	R^2	R	MSRE	R^2	R
T-varied	0.41	0.936	0.967	0.020	0.994	0.997
d-varied	0.37	0.961	0.980	0.018	0.996	0.998
B-varied	1.06	0.881	0.939	0.084	0.991	0.995
Fe-varied	0.06	0.991	0.996	0.005	0.999	0.999
All-varied	0.54	0.813	0.901	0.138	0.948	0.974

$\text{DNN}_{\text{FeFeB}}$ prediction is sufficiently large. But it should be noted, that the fraction of prediction with a big difference between $N_{\text{Fe,TRUE},i}$ and $N_{\text{Fe,PRED},i}$ is not numerous in most cases. Thus squared relative error (SRE) does not exceed 0.05 for 87%, 88%, and 96% samples from T-varied, d-varied and Fe-varid datasets respectively – see bars in Fig. 3. For the B-varied dataset (with doping level value, non-used in the training dataset) the biggest MSRE = 1.06 connects to the occurrence of some samples with a really big SRE (>20). While SRE is less than 0.05 in 54% of samples from the B-varied test dataset. The worst predictions are quite expectedly to be observed for the All-varied dataset: R^2 equals 0.813 and SRE is less than 0.05 for 18% only. On the other hand, the Fe-varied dataset is most similar to real demand. And determination and correlation coefficients are high enough (0.991 and 0.996) in this case.

The dependencies on DNN prediction error on SC parameters values are under consideration too – see Figs. 4– 7. These figures represent data for the training dataset, the results for test datasets are similar. Thus Fig. 4(a) shows that the considerable increase in prediction error value is observed at $T > 320$ K for $\text{DNN}_{\text{FeFeB}}$. So the maximum SRE is about 20 and the SRE is less than 0.01 for 55% of samples at $T = 340$ K (Fig. 4(c)). Whereas those values are equal to 0.02 and 83% at $T = 290$ K (Fig. 4(b)). It has been shown previously [53], that temperature rise causes the increase in the intrinsic recombination's contribution to an ideality factor. As a result, the sign of Shockley-Read-Hall (SRH) recombination in n value become less evident and DNN predictive ability falls.

As shown in Fig. 5, the SC base thickness does not influence the prediction error (mean value as well as relative frequency) practically. But one can see in Fig 2(c,d), that an ideality factor value depend on base thickness at constant N_{Fe} . Therefore d_p is a significant parameter for DNN training.

The predictive error rises sharply with doping level decrees – see Fig. 6(a). Thus maximum SRE is about 0.05 for $N_B = 10^{17} \text{ cm}^{-3}$ (Fig. 6(c)) whereas squared relative error is less than 0.05 for 56% of samples only for $N_B = 10^{15} \text{ cm}^{-3}$ (Fig. 6(b)). The hole occupation of the Fe-related level determines the SRH recombination efficiency. Accordingly to the Fermi-Dirac statistics, the probability of a hole occupation in a non-degenerate p -type semiconductor with full acceptor

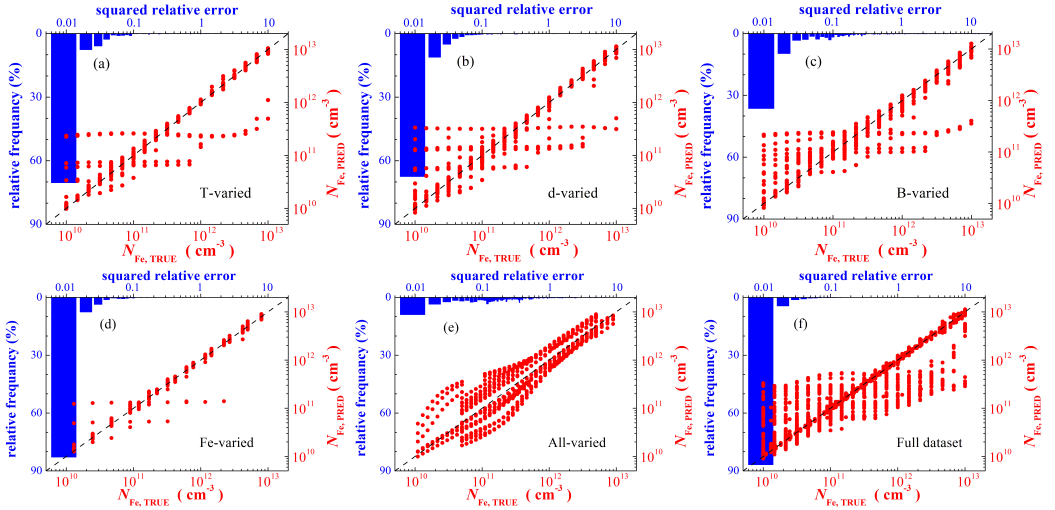


FIGURE 3 Iron concentrations are plotted against those generated by $\text{DNN}_{\text{FeFeB}}$ on T-varied (a), d-varied (b), B-varied (c), Fe-varied (d), All-varied (e), and full (f) datasets (red points). Bars represent histograms of squared relative error. DNN was learned by training (a)–(e) or full (f) dataset. The black dashed lines are the identify lines serving as the references.

depletion can be expressed as

$$f_p = \frac{1}{1 + \frac{N_V}{N_B} \exp\left(\frac{E_V - E_{Fe_i}}{kT}\right)}. \quad (12)$$

If N_B decreases, the level is filled with an electron, the SRH recombination ceases, and the ideality factor value sharply reduces — Fig. 2(a,b). Besides, a weak influence of impurities on ideality factor under low doping conditions is a reason for observed MSRE increase. In our opinion, the level filling is an additional reason for an error increase at high temperatures as well.

Fig. 7(a) shows that MSRE increases at both low and high iron concentrations. The first N_{Fe} area of bad DNN accuracy is entirely foreseeable, the second one is surprising enough. But accordingly to Fig 7(c), the MSRE increasing at $N_{\text{Fe}} = 10^{13} \text{ cm}^{-3}$ is most likely determined by a few samples with big SRE value. Whereas SRE increasing is more systematic at $N_{\text{Fe}} = 10^{13} \text{ cm}^{-3}$ — Fig 7(b).

The ideality factor value for the case of interstitial iron only presence (n_{Fe}) gives additional information about defects in comparing with $n_{\text{Fe-FeB}}$. It is not surprising that $\text{DNN}_{\text{FeFeB-Fe}}$ has better operating parameters in comparing with $\text{DNN}_{\text{FeFeB}}$ — see Table 3, Table 4, Fig. 8. The operation improvement appearances in the MSRE decrease as well as in absence of huge difference between $N_{\text{Fe,TRUE}}$ and $N_{\text{Fe,PRED}}$ values and narrowing of SRE range (Figs. 4-8). Really, it is shown in Fig. 8 that the maximum SRE does not exceed one even in the case of All-varied datasets and SRE is less than 0.02 for 93%, 92%, 73%, and 97% of samples of T-varied, d-varied, B-varied, and Fe-varied datasets respectively. The R^2 (0.999) and R (0.999) values for Fe-varied dataset draws attention as well.

Despite the difference in predicting accuracy, $\text{DNN}_{\text{FeFeB-Fe}}$ features are similar to $\text{DNN}_{\text{FeFeB}}$ ones. Thus the DNN training with N_B values, which are expected in object of future research, is important for prediction accuracy (Fig. 8); the increase in the temperature value (Fig. 4) as well as decrease in doping level (Fig. 6) or iron concentration (Fig. 7)

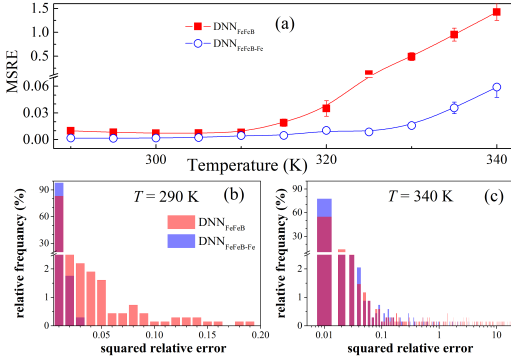


FIGURE 4 (a) Dependence of the MSRE (training dataset) on the temperature. (b),(c) Histograms of squared relative error for $T = 290$ K and $T = 340$ K. Red: DNN_{FeFeB}; blue: DNN_{FeFeB-Fe}.

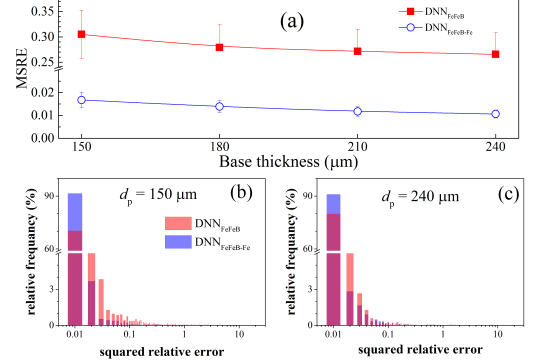


FIGURE 5 (a) Dependence of the MSRE (training dataset) on the base thickness. (b),(c) Histograms of squared relative error for $d_p = 150$ μm and $d_p = 240$ μm. Red: DNN_{FeFeB}; blue: DNN_{FeFeB-Fe}.

results in error rise. It should be noted that the prediction error gain with N_{Fe} increase not observed in DNN_{FeFeB-Fe} case and SRE range at $N_{Fe} = 10^{13} \text{ cm}^{-3}$ is more narrow then those at $N_{Fe} = 10^{10} \text{ cm}^{-3}$ — see Fig. 7(b,c).

The results of training both DNN_{FeFeB} and DNN_{FeFeB-Fe} with full dataset are presented in Table 3, Fig. 3(f), and Fig. 8(f). One can see that the extension of the labeled dataset does not practically improve the DNN result in our case. In our opinion, there is evidence of i) a good DNN configuration tuning; ii) a limited predictive ability of DNN_{FeFeB}, which caused by ambiguity of dependence $n_{Fe-FeB} = f(N_{Fe})$.

4.2 | Experimental IV curves

The ability of DNNs to predict the iron concentration in real silicon SCs was tested as well. The $n^+ - p - p^+ - \text{Si}$ samples were used in the experiment. The structures were fabricated from p -type boron doped Czochralski silicon wafer with [100] orientation and a resistivity of $10 \text{ Ohm} \cdot \text{cm}$ ($N_B = 1.4 \cdot 10^{15} \text{ cm}^{-3}$). The n^+ emitter with a sheet resistance of about $(20 \div 30) \text{ Ohm}/\square$ and a thickness of 0.7 μm was formed by phosphorus diffusion at 940°C . The p^+ layer $((10 \div 20) \text{ Ohm}/\square, 0.6 \text{ μm})$ was formed by boron diffusion at 985°C . The base thickness was equal to 350 μm . The samples used in the experiment had the area of $1.52 \times 1.535 \text{ cm}^2$. The concentration of iron in the SC base $N_{Fe,MEAS}$ was determined from kinetic of the short circuit current under monochromatic illumination [55]. Two samples, referred to as SC320 and SC349 with $N_{Fe,MEAS}$ values of $(2.0 \pm 0.4) \cdot 10^{12} \text{ cm}^{-3}$ and $(6.7 \pm 0.7) \cdot 10^{12} \text{ cm}^{-3}$, respectively, were used in the investigation.

One can see that DNN was faced with a rather difficult task, in which complexity is associated with a certain mismatch between the parameters of real structures and those used in the simulation. However, the need for iron-related defects, which predominantly determine recombination, was the main criterion for sampling in our case.

The dark $I - V$ characteristics of these samples were measured at temperatures of 300, 320, and 340 K. The measurements were taken after 48 h sample storage in the dark at room temperature ("Fe-FeB" case) as well as immediately after sample intense illumination with a halogen lamp ("Fe" case). After that, we used Eq. (10) to fit the experimental data and determine fitting parameters, in particular n , R_s , $R_s h$. The typical results of measurements and approximations are shown in Fig. 9 and Table 5. It should be noted that for real $I - V$ curves, in contrast to synthetic ones, the influence of series and shunt resistances cannot be neglected (the R_s values are about 3 and 6 Ohm for samples

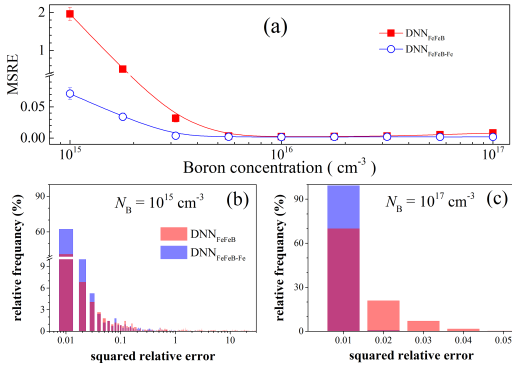


FIGURE 6 (a) Dependence of the MSRE (training dataset) on the boron concentration. (b),(c) Histograms of squared relative error for $N_B = 10^{15} \text{ cm}^{-3}$ and $N_B = 10^{17} \text{ cm}^{-3}$. Red: DNN_{FeFeB}; blue: DNN_{FeFeB-Fe}.

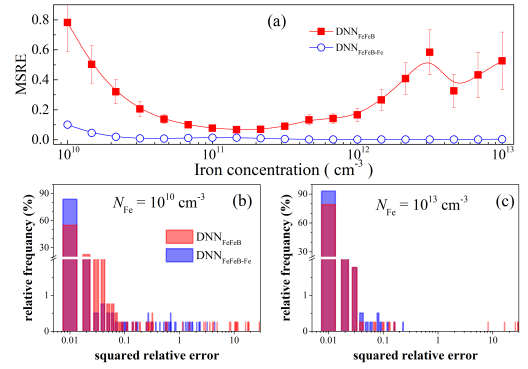


FIGURE 7 (a) Dependence of the MSRE (training dataset) on the iron concentration. (b),(c) Histograms of squared relative error for $N_{Fe} = 10^{10} \text{ cm}^{-3}$ and $N_{Fe} = 10^{13} \text{ cm}^{-3}$. Red: DNN_{FeFeB}; blue: DNN_{FeFeB-Fe}.

TABLE 5 Results of experimental IV fitting and iron contamination testing

Sample	$N_{Fe,MEAS}, 10^{12} \text{ cm}^{-3}$	$T, \text{ K}$	n_{Fe-FeB}	$R_{sh,Fe-FeB}, \text{ Ohm}$	n_{Fe}	$R_{sh,Fe}, \text{ Ohm}$	$N_{Fe,PRED}, 10^{12} \text{ cm}^{-3}$			
							DNN _{FeFeB}		DNN _{FeFeB-Fe}	
							training	full	training	full
SC320	2.0 ± 0.4	300	1.214	$1.6 \cdot 10^6$	1.195	$1.4 \cdot 10^6$	3.9	2.8	3.0	2.0
		320	1.204	$8.6 \cdot 10^5$	1.148	$8.0 \cdot 10^5$	6.6	1.9	16	19
		340	1.118	$4.3 \cdot 10^5$	1.111	$4.3 \cdot 10^5$	3.8	1.2	89	574
SC349	6.7 ± 0.7	300	1.223	$2.9 \cdot 10^6$	1.222	$2.6 \cdot 10^6$	8.9	5.6	15	11
		320	1.183	$1.7 \cdot 10^6$	1.182	$1.7 \cdot 10^6$	1.2	0.4	10	32
		340	1.138	$1.3 \cdot 10^6$	1.173	$1.3 \cdot 10^6$	9.8	1.7	26	411

SC320 and SC349, respectively, the Rsh values are listed in Table 5).

The values of the ideality factor, determined from the experimental curves, and the sample parameters were used as input data for DNN_{FeFeB} and DNN_{FeFeB-Fe}, which were trained on the training dataset or the full dataset. The predictions are listed in Table 5.

First of all, considering the not extreme high complexity of the simulation model, we note that the results even exceed expectations. Particularly for DNN_{FeFeB}, where the predicted iron concentrations differ by only several times from the measured ones. And in the case of sample SC320 and DNN_{FeFeB}, trained on the full dataset, the error does not exceed 40%.

Also, it should be noted that the results confirm the trends identified during analyzing synthetic $I-V$ curves. Namely, the prediction accuracy decreases for $T > 320 \text{ K}$ and iron concentrations, which are close to the upper limit of the considered range (10^{13} cm^{-3}). These facts fully coincide with the data in Fig. 4a and Fig. 7a, respectively. In addition, the sample's base doping level ($N_B = 1.4 \cdot 10^{15} \text{ cm}^{-3}$) is not used in the training dataset but can be found in the d-varied

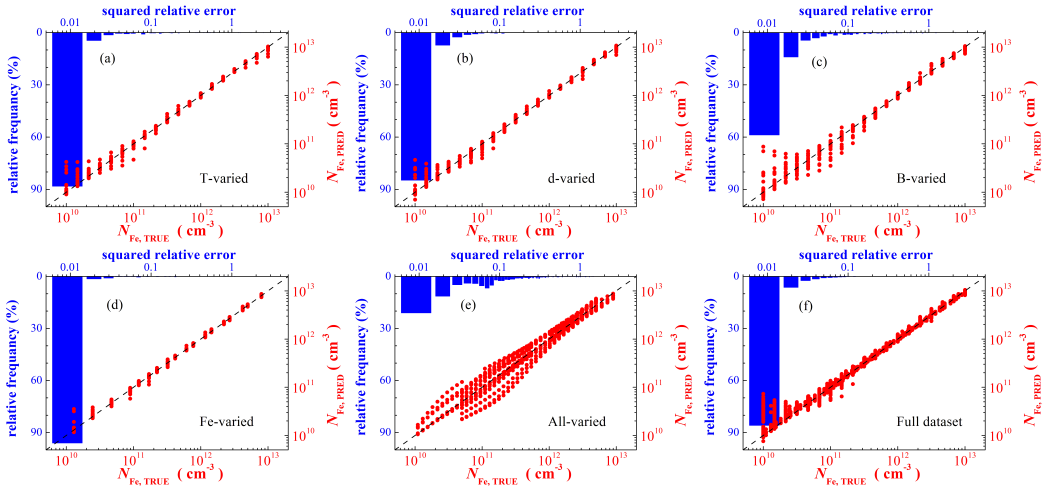


FIGURE 8 Iron concentrations are plotted against those generated by $\text{DNN}_{\text{FeFeB-Fe}}$ on T-varied (a), d-varied (b), B-varied (c), Fe-varied (d), All-varied (e), and full (f) datasets (red points). Bars represent histograms of squared relative error. DNN was learned by training (a)–(e) or full (f) dataset. The black dashed lines are the identify lines serving as the references.

dataset (see Supplementary Material). Table 5 shows that the prediction of $\text{DNN}_{\text{FeFeB}}$, trained by full dataset, is better than in the case of learning by training dataset only, especially for the SC320. This feature confirms the conclusion from the previous section about the importance of DNN training with N_B values, which are expected in the object of future research.

On the other hand, contrary to expectations, the $\text{DNN}_{\text{FeFeB-Fe}}$ demonstrate worse performance than $\text{DNN}_{\text{FeFeB}}$ in the case majority. There can be several reasons. Firstly, the use of two ideality factor values enhances the influence of simulation simplifications (e.g., the effect of unaccounted processes that cause the appearance of both shunt and series resistance). Secondly, the correct n_{Fe} determination is a more complicated experimental task than $n_{\text{Fe-FeB}}$ identifying. For example, it took about 100 s to obtain the I – V characteristics after intense illumination in our case. This interval consisted of time to set the temperature after illumination-induced heating as well as time to measurement. According to [43, 56], the characteristic association time of FeB pairs at $T = 340$ K and $N_B = 1.4 \cdot 10^{15} \text{ cm}^{-3}$ is about 600 s. Therefore, it cannot be expected that such a value of the ideality factor corresponds to the complete dissociation of FeB pairs. That is, despite the potentially higher accuracy of the $\text{DNN}_{\text{FeFeB-Fe}}$ predictions (shown in the previous section), the practical application of this approach is more complex.

Generally, the results obtained for real SCs confirm the possibility of estimation for iron contamination by ideality factor value.

5 | CONCLUSION AND OUTLOOK

In this paper, we extracted the iron concentration in silicon BSF solar cells from an ideality factor value and systematically studied the performance of deep learning in this problem. This work is the first attempt at using deep learning for deep levels parameter retrieval from the current–voltage curve. In this model study, we used simulation to obtain training and test labeled datasets. Besides, a DNN was trial-tested by using the parameters of actual solar cells. Our

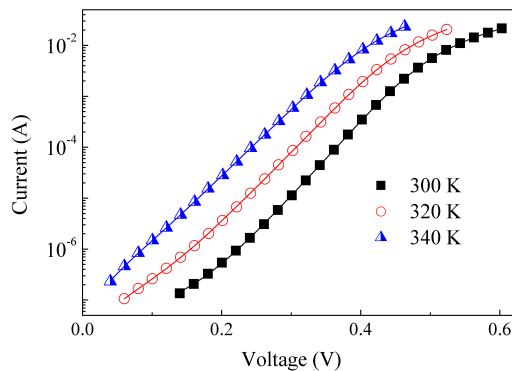


FIGURE 9 I – V characteristics measured at 300 K, 320 K, and 340 K for sample SC320. The marks are the experimental results, and the solid lines are the curves fitted by Eq. (10).

results showed the ability of the deep neural network to predict iron concentration by using ideality factor values, SC base thickness and doping level, and temperature. MSRE was up to 0.005 for synthetic datasets. The simulation has shown the prospects for the use of two ideality factor values (for structure with Fe_i only as well as with Fe_iB_s and Fe_i coexistence) for upgrading a prediction accuracy. At the same time, the practical application of such an approach manifested difficulties in obtaining correct data. It was important to train DNN with a boron concentration value, which agreed with the doping level of investigated structures. Moreover, the increase in iron concentration or boron concentration, as well as temperature decrease, results in a prediction error reduction.

The proposed approach envisages the utilization of a simple and widely applicable setup and does not require much time. Therefore it could be integrated into a manufacturing environment. However, it should be noted that we have simplified the task for our purposes. In our opinion, there are two ways of further improve the method. The first one connects with the refining of labeled datasets and can be realized by using 3D-simulators (e.g., SILVACO TCAD) or real IV measurements in a broad set of SCs. The improvement of DNN operation is the second one; and the fine-tuning is like most promising in this case. For example, not numerous input parameters can be multiplied and transformed to the picture and apply a vision model (e.g., VGG16).

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CONFLICT OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

DATA AVAILABILITY

The simulated IV characteristics, n_{Fe} and $n_{\text{Fe-FeB}}$ values, and trained DNNs are available at <https://github.com/olegolikh/IVcharacteristics.git>.

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