Dear editor,

We like to express our appreciation to the reviewers for their comments. We are resubmitting the revised version of the paper number PIP–21–281. We have studied the comments of the reviewer carefully, and have changed the text according to the comments they have listed. Below we refer to each of the reviewer's comments.

Response to Reviewer #1

Comment 1. *A solar cell with BSF is chosen as the basis of the work, claiming that "BSF is one of the popular designs used for industrial mass production...", but this is no longer the case, BSF solar cells are present in the market due to old manufacturing lines that are still operative, but the standard now is PERC technology. If the training of the network is based on SCAPS simulations, why was not trained with a PERC structure? At least, some hint on how results would be with a PERC structure should be given. (By the way, the BSF in this work is made with B-doping, which is also a minoritary approach at the industrial level, where BSF is of Aluminium).*

Reply: The Reviewer is absolutely right and PERC technology will be dominant in close future. But now the part of BSF solar cells is still big enough — see Fig. 1.

SCAPS-1D is a one-dimensional solar cell simulation program and the modeling of PERC solar cells with rear contact, which is inhomogeneous in a surface is a hard task. We understand the limitations of 1D simulators and noted this in the Conclusion.

We agree that it would be better to use Al-doped p^+-layer, but please consider the following. The simulated IV curves were used to obtain the ideality factor value n. According to the used two-diode model, n characterizes the current of second (so-called recombination) diode; the second diode current is due to recombination within the depletion region mainly [2, 3]. The p^+–layer influence on the mentioned process is rather determined by the pulling electric field. Therefore the kind of doping atom in the p^+–layer is not very important for our simulation. In the case of $n^+ - p - p^+$ structure with Al-doped base, the new training data set is needed, but the proposed deep-learning oriented approach to determining the impurity concentration remains valid. On the other hand, the recombination in the rear surface region is not dominant in n value determination. In our opinion, the trained DNNs can be applied to PERC solar cell in which i) the base is boron-doped; ii) the iron-related deep levels are the main reason for defect-assisted recombination.

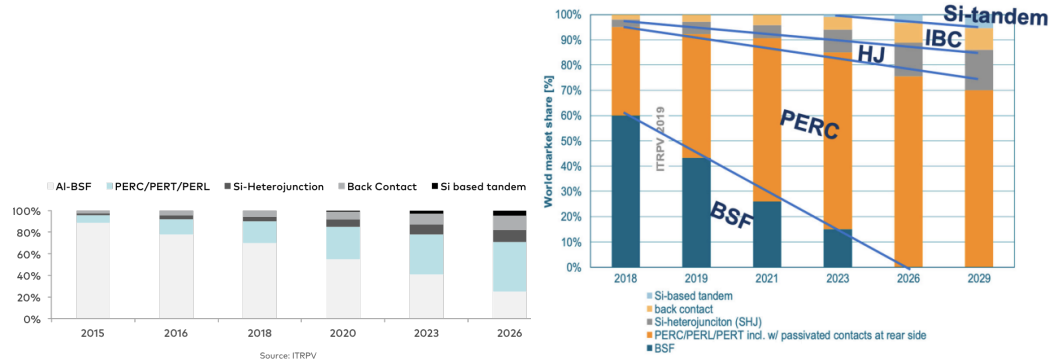

FIGURE 1 Projected manufacturing capacity share of different silicon–based cell technologies. Sources: https://www.aleo-solar.com/perc-cell-technology-explained/ (left panel), [1] (right panel).

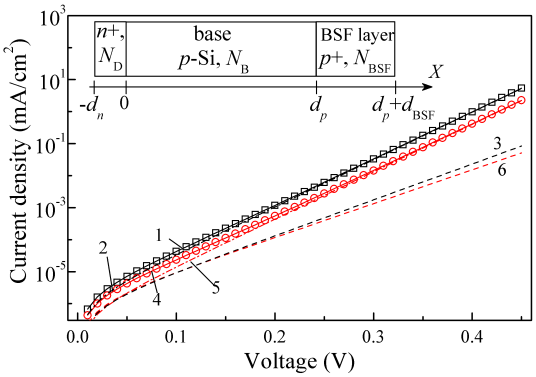

FIGURE 2 Simulated IV characteristic (marks) and its fitting by Eq. (1) (solid lines 1 and 4). The dashed (3, 6) and dotted–dashed (2, 5) lines represent the recombination diode currents and the "ideal" diode currents, respectively. $N_B = 10^{17}$ cm^{-3}, $N_{Fe} = 10^{13}$ cm^{-3}, $T = 340$ K, $d_p = 180$ μm. The results for Fe-case (circles, curves 4-6, red) and Fe-FeB case (squares, curves 1-3, black) are presented. Inset: Structures, which are used in the simulation.

The text was revised and some speculations about the applicability of the trained DNNs were added (last tree paragraph before Conclusion).

Comment 2. *As far as I understand, the simulation with SCAPS could be improved: emitter and BSF are uniform and this is not the case in reality. There is no mention to the metallization, are there no contacts? There should be, and they will influence the carrier transport and also the surface recombination velocities in the metal-semiconductor interface, among others.*

Reply: The flat bands' conditions were assumed for metal contacts on the rear and front surfaces. A sentence was added in the text. Let us note that it is common practice not to pay special attention in SCAPS simulation to contacts in the case of the barrier absence — e.g., see [4, 5, 6, 7, 8].

The Reviewer is correct about the way of SCAPS simulation improvement. In the present paper, we have concentrated on recombination in the SC base region, which mainly determines ideality factor value. The non-uniformities of emitter and BSF-layer affect much weaker on n value. In any case, the Reviewer's suggestion is very interesting and must be done in the future.

Comment 3. *Why a voltage sweep restricted to 0.45 V? This is rather low when compared to the voltages at the maximum power point of BSF solar cells... Wouldn't it influence in the extraction of the ideality factor values?*

Reply: We used the two-diode model to fit the simulated data. According to the two-diode model, the dark SC current is given by

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

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 the description of real Si SCs and the first diode represents the "ideal" diode and first term in Eq. (1) current is due to recombination in the base and the emitter, including their surfaces; the second diode is the so-called recombination diode and the second term is due to recombination within the depletion region [2].

The typical IV curves are shown in Fig. 2. It is seen that the contribution of recombination diode current is essential at low bias only. At $V \simeq 0.25$ V the first term in Eq. (1) is by an order of magnitude larger than the second one. A similar situation is observed for experimental IV curves — see Fig. 9 in Manuscript. The ideality factor value is related to the slope of recombination current dependence on voltage in a semi-logarithmic scale. Therefore the voltage range $(0 - 0.45)$ V is quite sufficient for an accurate determination of the ideality factor values.

The information was added on page 5, the first paragraph from the top.

Comment 4. *I am not sure that I interpret well the results in table 5. In the text the authors state that "the results even exceed expectations". But what I see is that the predictions fail in general, largely for the trained dataset cases, but also for the full dataset. There is some discussion on why* $DNN_{FeFeB-Fe}$ *performs worse than* DNN_{FeFeB} *and that is Ok... but* DNN_{FeFeB} *also fails in many cases, isn't it? (temperatures higher than 300K for the higher Fe content, 100% or more error for the training dataset...).*

Reply: On the one hand, the Reviewer is right. Unfortunately, the DNNs which was trained by synthetic data was disabled to measure iron concentration with extremely high precision in real solar cells (with a certain mismatch in their parameters and those used in the simulation). From this point of view "glass is half empty".

On the other hand, some reasons for "glass is half full" are present as well. First of all, in our opinion, the low cost express method which uses a widely applied setup and is able to approximate estimate the range of iron concentration (even with 100% error) can be useful. And the possible pathways for precision improvement are discussed in the Conclusion. Moreover, the results in Table 5 prompt the correct utilization of the proposed method in practice. Namely, the near room temperature of IV measurement is preferable (this conclusion is similar to those drawn from the analysis of synthetic IVs); the time between the pair dissociation and IV measurement must be as short as possible. Finally, in some cases (300 K, full dataset) the DNN_{FeFeB} yields acceptable results.

We hope that the use of deep learning for retrieval of deep level parameters from the current–voltage curve will find further development.

Comment 5. *In the jargon, we do not talk of surface resistance, but sheet resistance. Also, it is the first time that I read the "anti-recombination isotype barrier" for a high-low junction or a BSF.*

Reply: The Reviewer is absolutely right. We have revised the text accordingly.

Comment 6. *It is mentioned in the paper that there is Suplementary Material, but I have not had the opportunity to read it.*

Reply: We apologize for the embarrassment. But we are in confusion: Reviewer #2 mentioned the data in the table of Supplementary Material.

Comment 7. *On the other hand, the paper needs a thorough revision of English, preferably by a native or bilingual speaker. English is not my mother tongue, but I think that there are many expressions that are not correct, and make the reading difficult. From the abstract ("The low-cost and express...", "an ideality factor values"...) to the conclusions ("not numerous input parameters can be multiplied and transformed to the picture and apply a vision model..."(?), and a lot in between: "both for microelectronics, logic technologies and solar cells", "the various semiconductor barrier structures", "practical using", "Fours", "SFB", "in our further calculation", "simulated with using", "in comparing with", "more narrow", etc. etc.*

Reply: We are sorry for the English. The text was revised by the bilingual speaker, and we hope for language improvement.

Response to Reviewer #2

Comment 1. *2 Simulation details*

It is assumed that all SRH recombination in the device come from iron impurities and the associated deep level defects. It seems necessary to discuss its validity, and it could be interesting to put it against the fact that Al-BSF devices based on Czochralski silicon wafers are considered. More generally, if another type of defects is present in the solar cell, also inducing SRH recombination, is it possible to estimate to what extend are the DNNs trained here still accurate ?

Reply:

The speculations about the applicability of the trained DNNs to different SC structures must be based on assumption that the ideality factor distinguishes depletion-region recombination from most other sources of recombination [2, 3]. Certainly, there are some differences from this rule for real structures. For instance, our simulation reveals the n dependence on base thickness [9]. But this dependence is weak and the ideality factor value is mainly determined by depletion-region recombination nevertheless.

First of all, the DNNs applicability is related to the requirement of predominating of Shockley–Read–Hall recombination. In the cases of another mechanism of free carrier concentration decrease the models which diverge from two-diode is proposed (e.g., tree-diode [10, 11]). Moreover, the base must be doped by boron. For example, if SC is prepared from Si:Al wafer, the simulation model which is used for training dataset preparation must be modified: the parameters of Fe_iAl_s pair are needed to take into consideration as well as the changes of defect distribution (Eq. (**??**)). Finally, if another type of defect (in addition to iron–related deep levels) is present in the solar cell, also inducing intensive SRH recombination, the simulation model must be more complicated as well. The primary competitors of Fe_iB_s are boron-oxygen complexes [12, 13] and oxide precipitates [14, 15] in Cz-Si; and the corresponding model can be a next step. By the way, it is pertinent to note that the indicator of the presence of another defect can be a high n value: in our simulation $n < 1.4$ is observed. Last may be a most limiting factor of the DNNs applicability; in particular, it confined SCs selection for experimental verification of the proposed method.

Thus the trained DNNs can be applied to BSF solar cells prepared from Si:B wafers. It would be noted that the modern manufacturing technique allows to substantially restrict oxygen concentration in even Cz-Si. On the one hand, the Al is used to produce the doped p^+ region at the industrial level [1, 16]. But a boron BSF is one of the promising techniques for achieving high quality back contact [17, 18] and the p^+ layer, which is doped by boron, was under our consideration. On the other hand, the p^+–layer influence on the depletion-region recombination process is rather determined by the electric field. Therefore the kind of doping atom in p^+–layer is not very important for simulation, and in our opinion, the DNNs is applicable for Al BSF cell as well.

Some speculations were added (last tree paragraph before Conclusion).

Comment 2. *When Fe-FeB and Fe cases are presented, it could be clearer to provide very few more explanations on both types of defects, and the important fact that iron-boron pairs can be temporarily dissociated, providing the Fe case, through the heat treatment or high illumination already mentioned.*

Reply: The corresponding corrections were done on page 4, the third paragraph from the top.

Comment 3. *3 Deep neural network models*

*It is clear how the main training dataset is created, and how the 4 * 9 * 11 * 19 = 7524 IV curves are generated. However, the definition of the test datasets and the values for temperature, base thickness, iron concentration and doping level are not clear for each T-varied, d-varied, etc. test set.*

Reply: The sample of values used for the Fe-varied dataset was added (the last paragraph on page 5, the first paragraph on page 6)

Comment 4. *For instance, in the case of the T-varied test set, it is mentioned that the same base thickness, iron concentration and doping level values are used as in training dataset. However, 4 * 9 * 19 = 684 and the amount of 894 IVs can't be explained by multiplying with any number of temperature values. In Supplementary Material, the associated summary table do neither explain this value 894. More generally these tables are difficult to interpret. It is possible that the subset of 144 values for T-varied test has been duplicated.*

Reply: The Reviewer is right: i) the subset of 144 values for the T-varied test dataset has been duplicated; ii) Table in Supplementary Material has mistakes and is not clear. The correct values of d_p, N_B, and N_{Fe} were listed in Table, but we have some problems with addition and multiplication. We apologize for the inattention. The Table in Supplementary Material was revised.

Comment 5. *4 Results and discussion*

On figures 4, 5, 6 and 7, very interesting results are presented, and analyses of the dependence of estimation error with temperature, boron or iron densities and base thickness are well done. However, it seems that the same error statistics of results obtained on test datasets (instead of training dataset) would more directly assess the quality of predictions by the DNNs. For instance, the Fe-varied dataset has been identified to be the closest to "real demand" or results obtained with the all-varied dataset would also be most probably very useful. Such results could be showed in Supplementary Material, in the same form as figures 4, 5, 6 and 7.

Reply: The Supplementary Material was completed by figures (Figs. 8S–) which represent similar results for test datasets.

But it would be noted that error statistics for the training dataset are more correct and informative. For instance, let's consider temperature dependence (Fig. 4(a)). In fact, the averaging over 684 values was performed for each of 11 points in the training dataset. And this values correspond to data which uniformly distributed in range of used (N_{Fe}, N_B, d_p)-space.

In contrast, only 55 IV characteristics correspond to $T = 295$ K in the Fe-varied dataset (see Table in Supplementary Material). In the All-varied dataset 6 used values locate in range 290 – 315 K and only 3 values are in 315 – 340 K. Besides, 8 IV characteristics were simulated at $T = 293$ K for $N_{Fe} = (5 - 9) \times 10^{12}$ cm^{-3} (high values) whereas 60 ideality factor values are available at $T = 292$ K and $N_{Fe} = 1.1 \times 10^{12} - 5 \times 10^{12}$ cm^{-3} were used for simulation of corresponding IV curves.

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