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 programme and the modeling of PERC solar cells with rear contact, which is inhomogeneous, in surface is hard task. We understand the limitations of 1D simulators and noted about 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 used two-diode model, n characterizes current of second (so-called recombination) diode; the current of second diode current is due to recombination within the depletion region mainly [2]. The p^+–layer influence on mentioned process is rather determined by pulling electric field. Therefore the kind of doping atom in 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 DNN can be applied to PERC solar cell in wich i) the base is boron-doped; ii) the iron-related deep levels are the main reason of defect-assisted recombination.

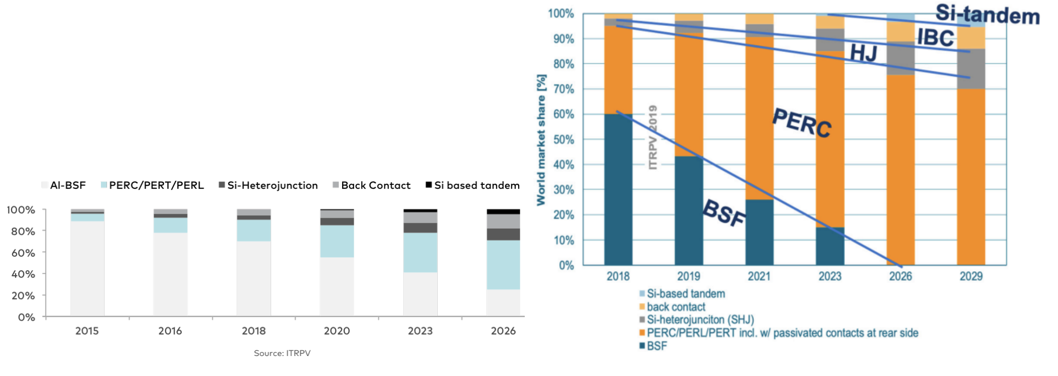

FIGURE 1 Projected manufacturing capacity share of different silicon–based cell technologies. Sources: https://www.aleo-solar.com/perc-cell-technology-explained/ (left panel), [1] (right panel).

The text was revised and the some information (hint) was added in page

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 on the rear and front surfaces. A sentence was added in 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 [3, 4, 5, 6, 7].

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 determine ideality factor value. The non-uniformities of emitter and BSF-layer affect much weaker on n value. But 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

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

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 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 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 term. Similar situation is observed for experimental IV curves — see Fig. 9 in Manuscript. The ideality factor value is related to slope of recombination current dependence on voltage in 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 in page

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...).*

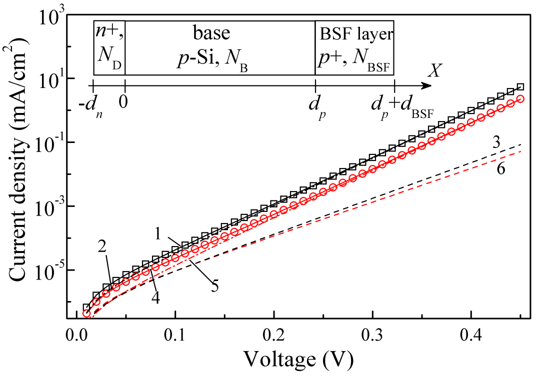

FIGURE 2 Simulated IV characteristic (marks) and its fitting by Eq. (1) (solid lines 1 and 4). The dashed (3, 6) and dotted–dashed (2, 5) lines represent the recombination diode currents and the "ideal" diode currents, respectively. $N_B = 10^{17}$ cm^{-3}, $N_{Fe} = 10^{13}$ cm^{-3}, $T = 340$ K, $d_p = 180\,\mu$m. 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.

Reply: The text was revised.

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 embarrassing. But we are in confusion: Reviewer #2 mentioned about 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 English. The text was revised by bilingual speaker and we hope for language improving.

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 text was revised.

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 in page

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 which used for Fe-varied dataset was added in page

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

REFERENCES

[1] Green MA. Photovoltaic technology and visions for the future. Prog Energy 2019 Jul;1(1):013001.

[2] Breitenstein O. Understanding the current-voltage characteristics of industrial crystalline silicon solar cells by considering inhomogeneous current distributions. Opto–Electronics Review 2013 Sep;21(3):259–282.

[3] Hu ET, Yue GQ, Zhang RJ, Zheng YX, Chen LY, Wang SY. Numerical simulations of multilevel impurity photovoltaic effect in the sulfur doped crystalline silicon. Renewable Energy 2015 May;77:442–446.

[4] Hamache A, Sengouga N, Meftah A, Henini M. Modeling the effect of 1 MeV electron irradiation on the performance of n^{+}-p-p^{+} silicon space solar cells. Radiat Phys Chem 2016 Jun;123:103–108.

[5] Cappelletti MA, Casas GA, Cédola AP, y Blancá ELP, Soucase BM. Study of the reverse saturation current and series resistance of p-p-n perovskite solar cells using the single and double-diode models. Superlattices Microstruct 2018 Nov;123:338–348.

[6] Azri F, Meftah A, Sengouga N, Meftah A. Electron and hole transport layers optimization by numerical simulation of a perovskite solar cell. Solar Energy 2019 Mar;181:372–378.

[7] Chowdhury MS, Shahahmadi SA, Chelvanathan P, Tiong SK, Amin N, Techato K, et al. Effect of deep-level defect density of the absorber layer and n/i interface in perovskite solar cells by SCAPS-1D. Results Phys 2020 Mar;16:102839.