

Dear Editor and Reviewers,

We sincerely thank you for taking the time to review our manuscript “Extracting the iron concentration in silicon solar cells using photovoltaic parameters and machine learning” (Ms. Ref. No.: SEJ-D-25-01089). Your insightful comments and constructive suggestions have greatly helped us improve the quality of our work. We particularly appreciate your careful reading and thoughtful feedback, which have led to significant improvements in both the technical content and presentation clarity of our manuscript. We have carefully addressed all the comments and made corresponding revisions to the manuscript. The location of revisions is pointed by red color and highlighted in yellow in “MarkedManuscript.pdf”. Below we provide our detailed point-by-point responses to each comment. We hope the revised manuscript better meets your expectations and standards for publication in Solar Energy.

Response to Reviewer #1

Comment 1. *The introduction lacks the role of iron valency (ferrous or ferric) in silicon solar cells.*

Reply:

Reviewer is correct that ferrous (Fe^{2+}) and ferric (Fe^{3+}) states deserve consideration, as they are the most common and stable charge states of iron. These ionic forms typically occur in compounds where iron forms chemical bonds (either ionic or covalent) with other elements, as well as in cases where iron is present as an impurity in solid materials. In silicon, iron can also exist in a trivalent (ferric) state when it substitutes for a silicon atom at a lattice site. However, under normal conditions, the concentration of substitutional iron is extremely low, less than 1% of the total iron impurity atoms [1]. Increasing the concentration of substitutional iron requires special sample processing, such as high-temperature annealing or irradiation. Moreover, substitutional iron acts as a weak recombination center, so its influence on the properties of silicon solar cells can be neglected. The ferrous form is virtually absent in silicon. The majority of iron impurity atoms in silicon occupy positions, where they can exist in either a neutral (Fe_i^0) or positively charged (Fe_i^+) state, depending on the position of the Fermi level [2]. In *n*-type silicon, Fe_i is more likely to exist in a neutral state, whereas in *p*-type silicon, it is more likely to be positively charged. Even when interstitial iron forms complex point defects, such as iron–boron pairs (Fe_iB_s), no valence bonds are formed. In interstitial configuration, iron acts as an active recombination center.

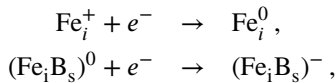
Consequently, in silicon solar cells, the role of iron valence is negligible, in contrast to other types of solar cells, such as perovskite solar cells [3]. Specifically, in MAPbI_3 -based devices, both Fe^{3+} and Fe^{2+} point defects are observed, with Fe^{3+} being electronically inactive in terms of recombination.

We have added the relevant information to the Introduction (page 2, third paragraph from the top).

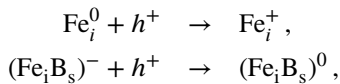
Comment 2. *The work didn't deal with the redox reaction of iron in silicon solar cells.*

Reply:

Initially, it is important to note that redox reactions do not play a central role in silicon solar cells, unlike dye-sensitized solar cells or photoelectrochemical cells. However, changes in the charge states of individual atoms — whether intrinsic or impurity-related — occur during the photoelectric conversion process. For example, during the recombination of charge carriers at iron-related defects (such as interstitial iron atoms or iron-boron pairs), electron capture occurs in the initial stage:



which typically corresponds to a reduction reaction. In the subsequent stage, hole capture alters the defect's charge state again



formally representing an oxidation reaction. When FeB pairs dissociate due to intense illumination, electron injection, or heating up to 200 °C, the iron atom becomes neutral by capturing an electron (reduction) during the first step of this two-stage process. After dissociation and the cessation of the external stimulus, the interstitial iron atom loses an electron (oxidation), becoming singly positively charged, which allows it to re-form a pair with a negatively charged

dopant (boron). However, transitions between different charge states of iron-related defects in silicon are governed by electron and hole capture and emission processes, involving the exchange of carriers between the defect levels and the conduction or valence band. These processes are described within Shockley–Read–Hall theory and do not constitute redox reactions in the classical chemical sense.

Consequently, the original manuscript did not emphasize redox reactions of iron in silicon solar cells, and the Reviewer's observation is valid. In the revised manuscript, we have included a note on the distinct nature of charge-state transitions in iron-related defects, highlighting how they differ from classical redox reactions (page 2, fourth paragraph from the top).

Comment 3. *In the title, "Extracting the iron concentration" should be changed to "Determination of iron concentration."*

Reply:

We concur that the phrase "Determination of iron concentration" better emphasizes the quantitative aspect of the work and aligns well with the standard terminology used in similar studies. Accordingly, we have revised the manuscript title to: "Determination of iron concentration in silicon solar cells using photovoltaic parameters and machine learning."

Response to Reviewer #2

Comment 1. *Why temperature range (290-340) K? what was the dissociation efficiency of FeB pairs at this temperature? How much is translated to cell degradation? Since at this temperature range, other factors also go side on that impact device characteristic.*

Reply:

We hope that the proposed approach will be applied to evaluate the concentration of iron in already installed solar modules and during the certification of photovoltaic converters. On the one hand, the selected temperature range of 290–340 K reflects the typical operating conditions of most silicon solar cells. On the other hand, the IEC 61215-2:2021 [4] standard requires that temperature coefficients of short-circuit current, open-circuit voltage, and maximum power be determined based on current–voltage measurements conducted within a temperature range of approximately +15 °C to +75 °C (288–348 K). In other words, the standard solar cell testing results can serve as input data for machine learning models trained within selected temperature range.

Additional information justifying the choice of temperature range has been added in the revised manuscript (page 4, first paragraph).

Complete dissociation of the FeB pairs was achieved during experiments conducted within the specified temperature range (further clarified below in response to the following Reviewer's comment).

The changes in photovoltaic parameter values resulting from FeB pair dissociation depend on both the concentration of iron impurities and the solar cell parameters (such as base thickness and dopant concentration), as well as the measurement conditions (illumination intensity and spectral composition, temperature). This issue is discussed in more detail in [5], which presents the results of silicon solar cell modeling used to create the training dataset. For instance, under AM1.5 illumination, the relative changes in short-circuit current range from –40.88% (for $N_B = 10^{17} \text{ cm}^{-3}$, $T = 290 \text{ K}$, $d_p = 380 \text{ }\mu\text{m}$) to 6.11% (for $N_B = 10^{15} \text{ cm}^{-3}$, $T = 315 \text{ K}$, $d_p = 380 \text{ }\mu\text{m}$). Similarly, the relative changes in open-circuit voltage vary from –12.95% (for $N_B = 10^{15} \text{ cm}^{-3}$, $T = 340 \text{ K}$, $d_p = 180 \text{ }\mu\text{m}$) to 1.92% (for $N_B = 1.778 \times 10^{15} \text{ cm}^{-3}$, $T = 340 \text{ K}$, $d_p = 230 \text{ }\mu\text{m}$). Notably, the most pronounced changes in solar cell characteristics do not necessarily occur at the highest iron concentrations. For example, the maximum negative change in open-circuit voltage (–12.95%) is observed at an iron concentration of $3.162 \times 10^{12} \text{ cm}^{-3}$, rather than at the highest tested level.

This suggests that FeB pair dissociation, depending on the specific parameters, can not only degrade solar cell performance but also improve certain characteristics [5, 6]. However, it is important to emphasize that light-induced dissociation of FeB pairs does not lead to irreversible changes in photovoltaic parameters. Once the illumination ceases, the FeB pairs re-form, and the solar cell characteristics return to their original values [7, 8, 9, 10, 7, 8].

Information regarding the ranges of changes in photovoltaic parameters and their reversibility has been added to the revised manuscript (page 4, third paragraph from the top; page 3, first paragraph in Section 2.1).

We fully agree with the Reviewer that, within the chosen temperature range, factors beyond iron concentration and the selected descriptors may also influence solar cell characteristics. This is especially relevant for real solar cells, which, in addition to iron, may contain other recombination-active impurities. To better isolate iron-related effects from the influence of other factors, we used relative changes in PV parameters as model inputs. Since models trained in this way provided sufficiently accurate predictions of iron concentration from both simulated and experimentally measured current–voltage characteristics, we consider this approach well justified.

Comment 2. *Complete details about the dissociation of FeB pairs using halogen lamp illumination? What was the time duration? How much was the decay efficiency.*

Reply:

It is known [11] that strong optical illumination ($>100 \text{ W/m}^2$) results in almost complete ($>99\%$) dissociation of the FeB pairs. The dissociation rate R_d is influenced by the pair concentration N_{FeB} and overall carrier generation rate G , which is proportional to the illumination intensity [7, 8, 9, 10]:

$$R_d = K \left(\frac{G}{N_{\text{FeB}}} \right)^2, \quad (1)$$

where K is the constant of the material. Additionally, it is well established that R_d depends on temperature [12, 13], the spectral composition of illumination [14], and the presence of recombination channels other than those associated with iron-related defects [7, 8].

For experimental validation of the proposed models, samples with an iron concentration of 2×10^{11} to $4 \times 10^{13} \text{ cm}^{-3}$ were used. Dissociation of FeB pairs was induced by intense illumination from a halogen lamp (7000 W/m^2). The illumination duration required to achieve near-complete dissociation depended on the iron concentration and reached up to 400 s for the solar cell with the highest N_{FeB} values. When selecting the illumination intervals, we considered the results of a previous study [14], which showed that in samples with a similar defect composition and exposed to a comparable light source, complete dissociation at $N_{\text{Fe}} = 9 \times 10^{12} \text{ cm}^{-3}$ occurred within 20 s.

Details regarding the selection of the illumination duration can be found on page 3 (last paragraph).

Comment 3. *Most of the models significantly fail for the AM1.5 illumination? What could be the reason for that?*

Reply:

Indeed, models trained on data obtained under AM1.5 illumination perform worse in almost all cases. We believe this can be attributed to the following reasons. It is well known that a regression model may achieve high accuracy by having the target variable be an unambiguous function of the descriptor. Moreover, the absolute value of the function's derivative should be as significant as possible. As shown earlier [5], the condition of uniqueness in the relationship between N_{Fe} and the changes in photovoltaic parameters under AM1.5 illumination is often not fulfilled in contrast to the case of monochromatic illumination. In addition, the ranges of changes in ϵI_{SC} , ϵV_{OC} , and $\epsilon \eta$ under monochromatic illumination exceed those observed under AM1.5 illumination. For illustration, Fig. 1 shows some examples from [5]. The physical origin of the differences in the relationship between iron concentration and parameter changes under AM1.5 and monochromatic illumination lies in the fact that, in the former case, the generation of non-equilibrium charge carriers occurs throughout the entire volume of the solar cell, rather than being limited to the base region. As a result, the processes involved in photovoltaic conversion are more complex. In our view, these differences explain why the performance of ML models trained on AM1.5 illumination data is generally poorer. One way to address the ambiguity in the relationship between features and the target variable is to incorporate additional features into the model. As shown in the study (e.g., see Fig. 7 in manuscript), for AM1.5 illumination, increasing the number of descriptors often improves prediction accuracy, supporting our hypothesis.

This answer is incorporated in the text on page 16, last paragraph and page 17, first paragraph.

Comment 6. *There are some typing mistakes as well. for e.g. Page 14, line 44, t-Itered...*

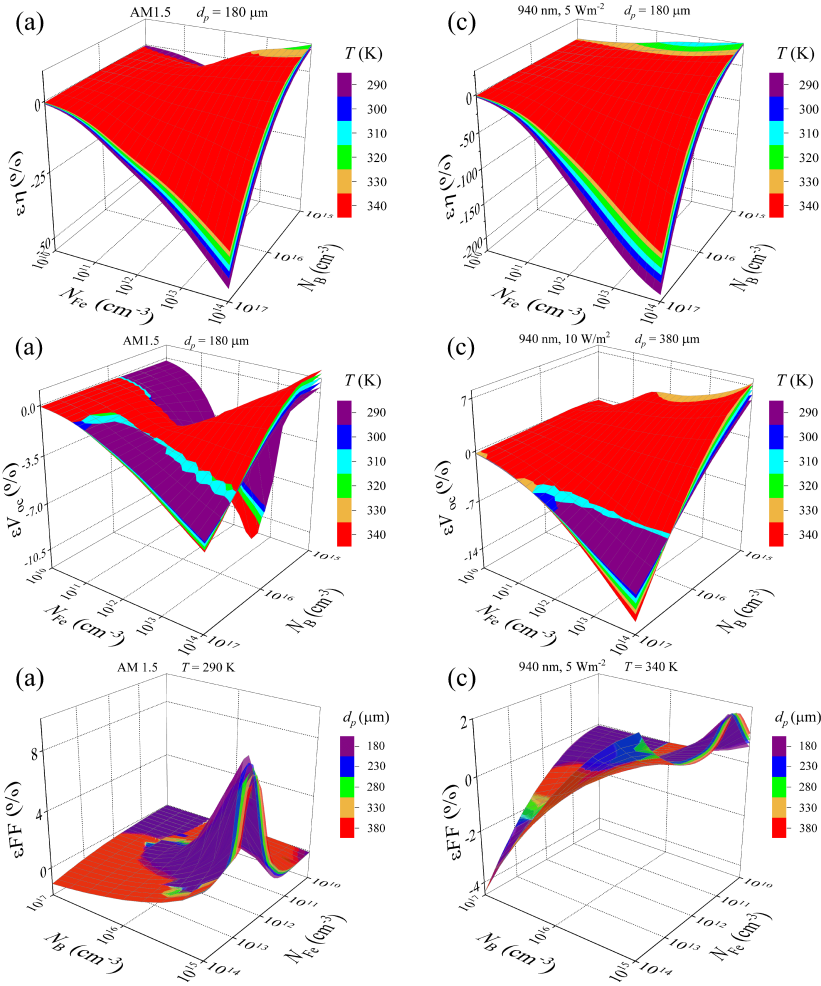


Figure 1: Relative changes in solar cell efficiency (first row), open-circuit voltage (second row), fill factor (third row) caused by a complete dissociation of Fe_iB_s . The dependencies are shown for two cases: AM1.5 illumination (left column) and 940 nm monochromatic light (right column). The figures are taken from reference [5].

Reply:

We thank the Reviewer for pointing out the typographical errors and apologize for their presence. We have carefully reviewed the entire manuscript and corrected typographical issues to improve its clarity and professionalism.

Comment 3. Table 1 and PCA does not add much value.

Reply:

In general, principal component analysis (PCA) is a widely used and effective tool in machine learning, particularly for addressing problems in photovoltaics. For example, it has been successfully applied to fault detection and classification based on I-V curves [15, 16], performance prediction of organic [17] and perovskite [18] solar cells, as well as measurement of the internal quantum efficiency in GaAs solar cells [19].

Despite previous successes in applying principal component analysis to various photovoltaics-related machine learning tasks — and the presence of favorable conditions for its use in our case, such as the high correlation between changes in photoelectric parameters caused by FeB pair dissociation — applying PCA as a data pre-processing step for evaluating iron impurity concentration did not improve the maximum prediction accuracy.

The inclusion of Table 1 and the PCA analysis was intended to transparently report our exploration of dimensionality reduction as a data pre-processing step. While our results show that PCA did not significantly improve model performance-and, in some cases, slightly reduced accuracy-we believe it is valuable to document that this common technique was systematically evaluated and found less effective than using the original features for this application.

We also note that, as the dataset size and feature space increase in future studies (for example, when modeling a wider range of device structures, operating conditions, or additional physical parameters), applying PCA or other dimensionality reduction methods could become more beneficial. In such cases, PCA can help reduce model training time and computational resources, as well as mitigate potential issues with feature redundancy and overfitting.

References

- [1] E. Wright, J. Coutinho, S. Öberg, V. J. B. Torres, Mössbauer parameters of fe-related defects in group-iv semiconductors: First principles calculations, *J. Appl. Phys.* 119 (2016) 181509.
- [2] A. A. Istratov, H. Hieslmair, E. Weber, Iron and its complexes in silicon, *Appl. Phys. A: Mater. Sci. Process.* 69 (1999) 13–44.
- [3] J. R. Poindexter, R. L. Z. Hoye, L. Nienhaus, R. C. Kurchin, A. E. Morishige, E. E. Looney, A. Osheroov, J.-P. Correa-Baena, B. Lai, V. Bulović, V. Stevanović, M. G. Bawendi, T. Buonassisi, High tolerance to iron contamination in lead halide perovskite solar cells, *ACS Nano* 11 (2017) 7101–7109.
- [4] IEC 61215-2:2021 - Terrestrial photovoltaic (PV) modules – Design qualification and type approval – Part 2: Test procedures, International Standard IEC 61215-2:2021, Geneva, Switzerland, 2021. <https://webstore.iec.ch/publication/61174>.
- [5] O. Olikh, O. Zavorodnii, Iron's impact on silicon solar cell execution: Comprehensive modeling across diverse scenarios, *Materials Science and Engineering: B* 317 (2025) 118192.
- [6] J. Schmidt, Effect of dissociation of iron–boron pairs in crystalline silicon on solar cell properties, *Progress in Photovoltaics: Research and Applications* 13 (2005) 325–331.
- [7] L. J. Geerligs, D. Macdonald, Dynamics of light-induced feb pair dissociation in crystalline silicon, *Appl. Phys. Lett.* 85 (2004) 5227–5229.
- [8] C. Möller, T. Bartel, F. Gibaja, K. Lauer, Iron-boron pairing kinetics in illuminated p-type and in boron/phosphorus co-doped n-type silicon, *J. Appl. Phys.* 116 (2014) 024503.
- [9] N. Khelifati, H. S. Laine, V. Vähänissi, H. Savin, F. Z. Bouamama, D. Bouhafs, Dissociation and formation kinetics of iron–boron pairs in silicon after phosphorus implantation gettering, *Phys Status Solidi A* 216 (2019) 1900253.
- [10] S. Herlufsen, D. Macdonald, K. Bothe, J. Schmidt, Imaging of the interstitial iron concentration in crystalline silicon by measuring the dissociation rate of iron–boron pairs, *Phys. Status Solidi RRL* 6 (2012) 1–3.
- [11] D. H. Macdonald, L. J. Geerligs, A. Azzizi, Iron detection in crystalline silicon by carrier lifetime measurements for arbitrary injection and doping, *J. Appl. Phys.* 95 (2004) 1021–1028.
- [12] J. Lagowski, P. Edelman, A. M. Kontkiewicz, O. Milic, W. Henley, M. Dexter, L. Jastrzebski, A. M. Hoff, Iron detection in the part per quadrillion range in silicon using surface photovoltage and photodissociation of iron-boron pairs, *Appl. Phys. Lett.* 63 (1993) 3043–3045.
- [13] K. Lauer, C. Möller, D. Debbih, M. Auge, D. Schulze, Determination of activation energy of the iron acceptor pair association and dissociation reaction, in: *Gettering and Defect Engineering in Semiconductor Technology XVI*, volume 242 of *Solid State Phenomena*, Trans Tech Publications Ltd, 2016, pp. 230–235.
- [14] O. Olikh, O. Datsenko, S. Kondratenko, Influence of illumination spectrum on dissociation kinetics of iron–boron pairs in silicon, *Phys. Status Solidi A* 221 (2024) 2400351.
- [15] S. Fadhel, C. Delpha, D. Diallo, I. Bahri, A. Migan, M. Trabelsi, M. Mimouni, PV shading fault detection and classification based on I-V curve using principal component analysis: Application to isolated PV system, *Sol. Energy* 179 (2019) 1–10.
- [16] W. Gao, R.-J. Wai, A novel fault identification method for photovoltaic array via convolutional neural network and residual gated recurrent unit, *IEEE Access* 8 (2020) 159493–159510.
- [17] T. W. David, G. A. Soares, N. Bristow, D. Bagnis, J. Kettle, Predicting diurnal outdoor performance and degradation of organic photovoltaics via machine learning; relating degradation to outdoor stress conditions, *Prog. Photovoltaics Res. Appl.* 29 (2021) 1274–1284.
- [18] Y. Liu, W. Yan, S. Han, H. Zhu, Y. Tu, L. Guan, X. Tan, How machine learning predicts and explains the performance of perovskite solar cells, *Sol. RRL* 6 (2022) 2101100.
- [19] Z. Abdullah-Vetter, B. Wright, T.-C. Wu, A. Shakiba, Z. Hameiri, Automatic quantitative analysis of internal quantum efficiency measurements of gaas solar cells using deep learning, *Adv. Sci.* 12 (2025) 2407048.