

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.

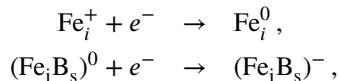
Consequently, in silicon solar cells, the role of iron valence is negligible, in contrast to other types of solar cells, such as perovskite solar cells [3]. Specifically, in MAPbI_3 -based devices, both Fe^{3+} and Fe^{2+} point defects are observed, with Fe^{3+} being electronically inactive in terms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

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

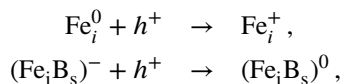
Comment 2. *The work didn't deal with the redox reaction of iron in silicon solar cells.*

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 [8, 9, 10, 11, 8, 9].

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 [7] 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 [8, 9, 10, 11]:

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

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 [8, 9].

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:

The reduced accuracy of most models under AM1.5 illumination likely results from the increased complexity of the broadband solar spectrum compared to monochromatic light. Under AM1.5, the photovoltaic parameter changes are influenced by a wider range of physical effects and interactions, making the relationship between input features and iron concentration more complex and less direct. This complexity makes it more challenging for many models-especially simpler ones-to generalize well, even when trained on simulated data. In contrast, monochromatic illumination provides a more straightforward correlation between iron-related recombination and PV parameter changes, resulting in higher model accuracy.

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

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.

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.

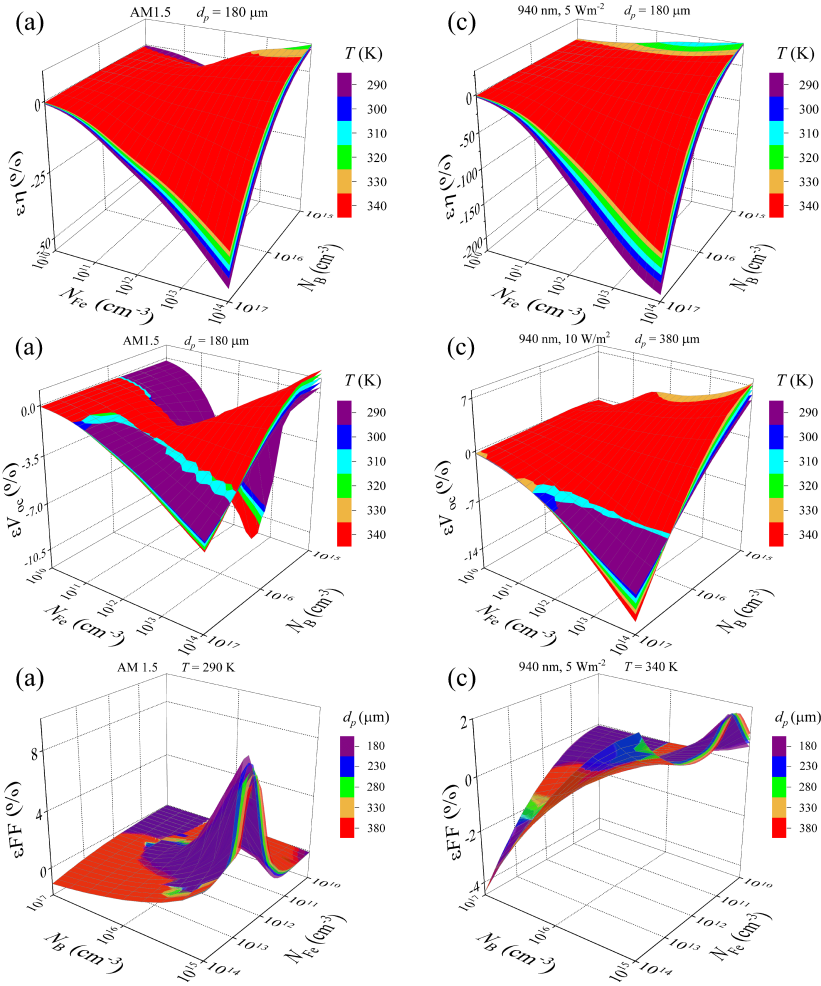


Figure 1: Relative changes in solar cell efficiency (first row), open-circuit voltage (second row), fill factor (third row) caused by a complete dissociation of Fe_iB_s . The dependencies are shown for two cases: AM1.5 illumination (left column) and 940 nm monochromatic light (right column). The figures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

- [3] J. R. Poindexter, R. L. Z. Hoye, L. Nienhaus, R. C. Kurchin, A. E. Morishige, E. E. Looney, A. Osherov, 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] 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.
- [8] L. J. Geerligs, D. Macdonald, Dynamics of light-induced feb pair dissociation in crystalline silicon, *Appl. Phys. Lett.* 85 (2004) 5227–5229.
- [9] 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.
- [10] 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.
- [11] 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.
- [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.