Dear Editor and Reviewers,

We sincerely thank you for taking the time to review our manuscript "Iron's impact on silicon solar cell execution: comprehensive modeling across diverse scenarios" (Ms. Ref. No.: MSB-S-24-02710). 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. 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 Materials Science and Engineering: B.

Response to Reviewer #1

Comment 1. *The author must explain the specific mechanisms you propose for the interaction between iron-related defects and other impurities in silicon solar cells? How might these interactions complicate the interpretation of photovoltaic performance metrics?*

Reply:

In general, interstitial iron is already mobile at room temperature and can interact with various impurities. Over 30 iron-related complexes have been identified in silicon, and nearly 25 energy levels associated with iron-related defects have been reported in the silicon bandgap across different studies [1, 2, 3]. For example, iron forms complexes with carbon, oxygen, hydrogen, sulfur, and other metal impurities, as well as with native defects in silicon. However, in terms of their impact on photovoltaic performance, two primary factors must be considered. First, the concentration of the relevant defects is crucial. It is widely recognized that in p–type silicon under equilibrium conditions, most iron impurity atoms pair with acceptors (e.g., boron in Si:B) [4, 1]. The concentration of other complexes is significantly lower, and detailed investigation of these complexes requires specialized sample preparation, such as additional doping with other expected complex components or irradiation to increase the concentration of native defects [5]. Further supporting this, several methods used to evaluate the total iron concentration in p–Si rely on breaking the FeB pair [6, 7, 8]. Second, the recombination activity of these centers must be considered, as it depends on the defect energy level relative to the Fermi level and the charge carrier capture cross-section. Interstitial iron and FeB pairs are among the most detrimental recombination-active impurities in p–Si [1, 9] in contrast to other iron-related defects. Notably, iron gettering by oxygen precipitates or structural defects increases carrier lifetime [10, 11]. In n–Si, Fe_i is not a recombination-active impurity due to the filling of its energy level. Reducing the impact of iron through gettering during phosphorus diffusion [10, 11, 12] or the formation of a passivating layer [13] is well-established and used in the solar cell industry.

Thus, our assumption that the primary influence of iron impurities in the p–regions of a solar cell on photoelectric parameters is due to Fe_iB_{Si} pairs and Fe_i is fully justified. Furthermore, we emphasize that this paper focuses on the relative changes in parameters during $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ transformation, which enables the isolation of these specific defects' contributions.

This answer is incorporated in the revised text on page 5, two last paragraph in Section 2.1. Simulation Details.

Comment 2. *The author should give the transient nature of defect dynamics, how do you assess the long-term stability of silicon solar cells in the presence of iron contamination? What experimental approaches would you recommend to study the aging effects of these defects over time?*

Reply:

Interstitial iron atoms exhibit high mobility in silicon [1]. For example, the characteristic time required for FeB pair formation, which depends on the diffusion coefficient of Fe_i, is given by the following expression [14, 15, 16]:

$$\tau = 5.7 \times 10^5 \, \frac{s}{K \, cm^3} \times \frac{T}{N_B} \exp\left(\frac{0.65}{kT}\right) . \tag{1}$$

where N_B is the doping level.

That is, at room temperature, the formation of an equilibrium concentration of FeB pairs is completed within 24 hours, while at $T = 340$ K, the τ is approximately 10 minutes. Therefore, iron contamination is not a determining factor in the long–term stability of silicon solar cells, unlike sodium atoms, which are considered one of the primary contributors to potential-induced degradation [17].

The information on the characteristic time of FeB pair formation has been added to the revised manuscript (page 5, last paragraph in Section 2.2.).

> The measurements were carried over the temperature range of 300-340 K. The sample temperature was driven by a thermoelectric cooler controlled by an STS-21 sensor and maintained constant by a PID algorithm embedded in the software that serves the experimental setup. Notably, the characteristic time for FeB pair recovery after the cessation of illumination is approximately 13,000 seconds at 300 K and only 600 seconds at 340 K [14, 15]. These limitations affect the measurement duration at high temperatures, and the experiments accounted for them.

Comment 3. *An Author should provide a theoretical framework for understanding how the temperature range you studied (290 K to 340 K) influences the activation energy of iron-related defects? How might this affect the performance of solar cells in varying environmental conditions?*

Reply:

Initially, we note that the selected temperature range reflects the realistic operating conditions of most silicon solar cells. In our calculations, we accounted for the temperature dependencies of both silicon properties — including bandgap, the effective density of states; effective masses, thermal velocities and mobilities of charge carriers; Auger and band-to-band recombination coefficients, and light absorption values — and defect parameters, such as energy level positions within the bandgap and electron and hole capture cross-sections. Additionally, we considered the temperature dependence of the equilibrium concentration ratio of Fe_i and FeB. Specifically, the primary effect of increasing temperature on iron-related defects is the rise in the relative equilibrium concentration of interstitial iron atoms and the change in the charge carrier capture cross-section of each defect.

Accounting for all the above factors in the modeling process suggests that the results presented in this work accurately reflect the impact of both defects and defect parameter variation on solar cell performance under varying environmental conditions, including temperature, illumination type, and intensity.

Details on how temperature dependencies were accounted for in the simulation can be found on page 3, last two paragraphs

> As can be seen from Table 1, calculations spanned a broad range of temperatures and base doping levels. Therefore, to improve the accuracy of the calculations when inputting the initial parameters into SCAPS, temperature and concentration (where applicable) dependencies of the following silicon parameters were taken into account:
> - bandgap according to Passler [18];
> - doping induced bandgap narrowing according to Yan & Cuevas [19];
> - effective density of states at conduction and valence band and intrinsic carrier concentration according to Couderc et al. [20];
> - thermal carrier velocities according to Green [21];
> - free carrier effective masses according to O'Mara et al. [22];
> - carrier mobilities according to Klaassen's theory [23];
>
> The values of surface recombination coefficients were considered equal to the thermal velocities of carriers [24]. The calculations addressed recombination processes within the structural volume, incorporating both intrinsic recombination and Shockley-Read-Hall (SRH) recombination at iron-related defects. In the first case, processes of band-to-band radiation recombination were considered (where the calculation of the corresponding coefficient included the fraction of radiatively emitted photons reabsorbed via band-to-band processes according to Niewelt et al.[25]) and Auger recombination (where the coefficients considered the effect of Coulomb enhancement [26] and temperature dependence [27]).

and page 4, 3rd and 4th paragraph from the top

Case 2. Iron atoms predominantly form pairs with acceptors, $[\text{Fe}_i\text{B}_s] \gg [\text{Fe}_i]$, but the exact concentration ratio depends on the position of the Fermi level and temperature [28, 29] and varies from point to point within the solar cell. Further details about calculation of the concentration profiles of Fe_iB_s and Fe_i are provided in [30, 31]. This case corresponds to prolonged storage of the structure in darkness or under conditions of low-intensity (< 0.01 J cm^{-2} [32]) illumination.

During the calculations, it was assumed that Fe_i forms a single donor level, while the Fe_iB_s pair has a trigonal configuration and acts as an amphoteric defect. We obtained defect parameters, including energy level positions within the bandgap, electron and hole capture cross-sections, and their temperature dependencies, based on data from relevant studies [33, 1, 34].

Comment 4. *An Author mentioned the application of principal component analysis in evaluating impurity levels. Could you elaborate on how this technique was implemented in your study and its effectiveness in distinguishing between different types of impurities?*

Reply:

One of the objectives of this study was to evaluate the feasibility of using variations in short-circuit current, open-circuit voltage, solar cell efficiency, or fill factor, which results from the decay of iron-containing pairs, to estimate the concentration of iron impurities. Our simulations revealed that the relative changes in these parameters depend not only on the iron concentration but also on temperature and other solar cell characteristics, such as doping level and base thickness. In other words, when determining the magnitude of N_{Fe} based on changes in short-circuit current, a set of parameters (descriptors) must be used: $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}})$. Evidently, incorporating additional information, such as changes in efficiency ($\varepsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$, increases the complexity of calculations due to the growing number of input parameters. However, this should enhance the accuracy of N_{Fe} predictions. Meanwhile, variations in short-circuit current and efficiency are not entirely independent, as both essentially characterize the same physical process — the diffusion of photo-induced carriers. Confirmation of this has resulted from analyzing the correlations between parameters — see Fig. 12 in the manuscript. Thus, the set $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}})$. To assess the degree of redundancy in different descriptor sets, we employed principal component analysis (PCA), which constructs a new dataset of uncorrelated principal components (PCs). PCA also enables the evaluation of each PC's contribution to the total variance of the information. Our analysis showed that, for example, when estimating N_{Fe} using a set of seven descriptors $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}}, \varepsilon\eta, \varepsilon V_{\text{OC}}, \varepsilon FF)$ obtained under 940 nm illumination, five PCs account for more than 99.5% of the variance in the input data. Therefore, applying PCA to transform the seven input variables and using only five is fully justified, as it significantly simplifies calculations with minimal impact on estimation accuracy.

In the manuscript, PCA was not used to evaluate impurity levels. The conclusions and abstract only mentioned its potential usefulness in estimating the concentration of iron impurities based on variations in several photovoltaic parameters. We apologize for any possible ambiguities in the wording. In the revised manuscript, we have aimed for the most precise formulations. Finally, we would like to thank the Reviewer for an idea about PCA use to distinguish the contributions of different defects in future research.

The corrections were made in the manuscript on page 15, 1st paragraph in Section 3.5.

The previous subsections demonstrated that by using the relative changes in photovoltaic energy conversion parameters following the dissociation of FeB pairs (e.g., changes in short-circuit current), along with considering solar cell parameters (such as base depth and doping level) and measurement conditions (such as temperature and illumination type), it is possible to predict iron concentration. One approach to evaluating the value of N_{Fe} is to apply a machine learning algorithm (random forest, gradient booster, or artificial neural network etc.). If we assume that the training process is conducted separately for each illumination variant and want to determine the magnitude of N_{Fe} based on changes in short-circuit current, the input set of descriptors could be $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}})$. Evidently, incorporating additional information, such as changes in efficiency ($\varepsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_\text{B}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$, increases the complexity of calculations due to the growing number of input parameters. However, this should enhance the accuracy of N_{Fe} predictions. At the same time, when comparing Fig. 3 and Fig. 10, it is clear that $\varepsilon I_{\text{SC}}$ and $\varepsilon\eta$ are not entirely independent. This outcome is understandable

from a physical standpoint as short-circuit current and efficiency characterize the same physical process — the diffusion of photo-induced carriers. Thus, the set $(T, d_p, N_B, \varepsilon I_{SC}, \varepsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_B, \varepsilon I_{SC})$.

and on page 15, two last paragraph

To assess the degree of redundancy information in different descriptor sets, we employed principal component analysis (PCA), widely used in solving various problems, including identifying defects in solar cells [35]. PCA uses a linear combination of the original variables to construct the new variables (principal component, PC) while keeping maximum variance information. PCs are uncorrelated, and PCA allows one to evaluate each PC's contribution to the total variance of the information. In the case of some particular principal component having a low information variance ratio, it can be discarded with little to no loss of useful information.

PCs were built for different combinations of photovoltaic parameters and solar cell characteristics for the full set of simulated data, and the results are listed in Table 2. As evident, when only changes in short-circuit current are considered along with the solar cell's base parameters and temperature, no excessive information is present (in the case of the descriptor set $(T, d_p, N_B, \varepsilon I_{SC})$, all four principal components exhibit a high ratio of information variance). And vice versa, when estimating N_{Fe} using a maximal set of seven descriptors $(T, d_p, N_B, \varepsilon I_{SC}, \varepsilon\eta, \varepsilon V_{OC}, \varepsilon FF)$ obtained under monochromatic illumination five PCs account for more than 99.5% of the variance in the input data. Therefore, applying PCA to transform the seven input variables and using only five is fully justified, as it significantly simplifies calculations with minimal impact on estimation accuracy. For the same set of descriptors obtained under AM1.5 illumination, the number of really independent variables is six. In general, if the estimation of iron concentration is based on changes in multiple photovoltaic parameters, it is advisable to apply PCA to transform the original data. Thus, the simultaneous use of $\varepsilon\eta$ and εI_{SC} practically does not alter the number of independent variables (four) compared to the initial set of descriptors. With the additional use of εV_{OC} values obtained under AM1.5 illumination, it is advisable to consider five independent variables. For the same set of descriptors in a monochromatic illumination case, one can limit oneself to using only four independent components (cumulative variance ratio for PC4 and PC5 does not exceed 1.3%).

Comment 5. *Your paper discusses the influence of doping levels on the response of solar cells to iron contamination. Author should explain how varying the doping concentration affects the sensitivity of photovoltaic parameters to iron presence through the reference: Augmented photovoltaic performance of Cu/Ce-(Sn: Cd)/n-Si Schottky barrier diode utilizing dual-doped Ce-(Sn: Cd) thin films.*
Reply:
The primary reason doping concentration N_B influences the sensitivity of photovoltaic parameters to iron presence is that the N_B determines the Fermi level E_F position. In turn, the rate of Shockley-Read-Hall recombination — and consequently, variations in photovoltaic parameters due to iron impurities — depends on the relative positioning of E_F concerning the Fe_iB_s and Fe_i levels. Additionally, the equilibrium ratio of Fe_iB_s and Fe_i concentrations is also determined by the Fermi level position [28, 29]. Therefore, N_B affects the number of defects that change their state due to the complete dissociation of Fe_iB_s pairs, leading to corresponding relative changes in photovoltaic parameters analyzed in this study. Besides, the N_B concentration also affects the SCR depth (see Fig. 4 in manuscript). The ratio of different charge states for both interstitial iron atoms and iron-boron pairs differs between the SCR and the bulk of the base, leading to distinct SRH recombination rates and variations in photovoltaic conversion efficiency for structures with different doping levels. Furthermore, according to Klaassen's model [23], the concentration of ionized impurities influences charge carrier mobility and, consequently, the diffusion coefficient D_n, diffusion length L_n, and photoelectric conversion efficiency (see Eqs. (4), (5), and (7) in the manuscript). However, the effect of N_B via D_n and L_n is significantly weaker than its influence through E_F and SCR depth variations. Minor effects are expected as well due to both bandgap narrowing and changes in light absorption by free carriers with varying doping levels. The impact of doping level on photovoltaic parameters has been studied in heterojunction [36], thin-film [37], and perovskite [38] solar cells. Moreover, it has been shown [37] that doping concentration variations affect other barrier structure parameters, such as saturation current and ideality factor.

This answer is incorporated in the text on page 4, paragraph 4, line 1-2. Reference is included in the revised manuscript (references 1)

...while the presence of the acceptor state Fe$_i$B$_s$ causes the carrier lifetime to be doping-dependent under low injection conditions [FeB:Schmidt].

The relationship between N_B and E_F is the key factor in the influence of doping level on the sensitivity of photovoltaic parameters to iron presence. Specifically, the rate of SRH recombination — and consequently, variations in photovoltaic parameters due to iron impurities — depends on the relative positioning of E_F concerning the Fe$_i$B$_s$ and Fe$_i$ levels. Additionally, the equilibrium ratio of Fe$_i$B$_s$ and Fe$_i$ concentrations is also determined by the Fermi level position [FeB:kinetic,MurphyJAP2011]. Therefore, N_B affects the number of defects that change their state due to the complete dissociation of Fe$_i$B$_s$ pairs, leading to corresponding relative changes in photovoltaic parameters analyzed in this study. Besides, the N_B concentration also affects the SCR depth (see Fig. 4). The ratio of different charge states for both interstitial iron atoms and iron-boron pairs differs between the SCR and the bulk of the base, leading to distinct SRH recombination rates and variations in photovoltaic conversion efficiency for structures with different doping levels. Furthermore, according to Klaassen's model [KLAASSEN953], the concentration of ionized impurities influences charge carrier mobility and, consequently, the diffusion coefficient D_n, diffusion length L_n, and photoelectric conversion efficiency (see Eq. (4)). However, the effect of N_B via D_n and L_n is significantly weaker than its influence through E_F and SCR depth variations. Minor effects are expected as well due to both bandgap narrowing and changes in light absorption by free carriers with varying doping levels. The impact of doping level on photovoltaic parameters has been studied in heterojunction [8], thin-film [10], and perovskite [6] solar cells. Moreover, it has been shown [10] that doping concentration variations affect other barrier structure parameters, such as saturation current and ideality factor.

Comment 6. *In your findings, Author mentions that changes in short-circuit current under monochromatic illumination are the most reliable for estimating iron concentration. An author should provide more details on the methodology used to derive this conclusion and any potential limitations of this approach?*

Reply:

We employed two key metrics to identify the solar cell parameter whose changes, resulting from the Fe$_i$B$_{Si}$ $\rightleftarrows$ Fe$_i$ + B$_{Si}$ reconstruction, enable the most reliable determination of iron concentration. Specifically, these metrics are: (1) the monotonicity of the relative change in the parameter value as a function of impurity concentration, which is a necessary condition for the unambiguous estimation of N_{Fe}; and (2) the absolute magnitude of the parameter change, which allows for more precise measurements and, consequently, a more accurate estimation of N_{Fe}. The first criterion is not satisfied by εFF, εV_{OC}, and $\varepsilon \eta$ (the latter two under AM1.5 illumination). At the same iron concentration, εI_{SC} values under monochromatic illumination exceed those under AM1.5 illumination. As mentioned earlier, this effect deals with differences in the generation locations of non-equilibrium carriers under different lighting conditions. Additionally, under identical conditions, the changes in open-circuit voltage are significantly weaker than those in short-circuit current or efficiency. Since εI_{SC} and $\varepsilon \eta$ are of the same order, it is advisable to select the more reliable parameter using additional metrics. Notably, short-circuit current determination, unlike efficiency, does not require additional calculations and can be directly extracted from the raw measured I-V curves. Furthermore, εI_{SC} is virtually independent of illumination intensity (whereas $\varepsilon \eta$ exhibits a weak dependence), leading to two key advantages: (a) iron concentration can be determined using an uncalibrated for-intensity monochromatic light source; (b) the influence of shading caused by electrodes, along with the antireflective and passivating layers of the solar cell, is reduced.

Thus, short-circuit current is the most suitable parameter for estimating the concentration of iron impurities, as its changes during the Fe$_i$B$_{Si}$ $\rightleftarrows$ Fe$_i$ + B$_{Si}$ transformation can be effectively utilized. Determining photovoltaic parameters under monochromatic illumination, with a wavelength corresponding to the predominant absorption in the solar cell base, is more effective than using AM1.5 illumination. The most viable alternatives are solar cell efficiency and open-circuit voltage; however, their applicability is limited at low base doping levels ($< 10^{16}$ cm^{-3}) due to non-monotonic variations in response to increasing iron concentration. In our view, using the fill factor for iron concentration estimation is impractical. These conclusions are validated by experimental results, which show that short-circuit current provides the most accurate determination of iron concentration.

The limitations of the proposed method may arise from the presence of a significant number of recombination-active defects unrelated to iron, as well as high series resistance (which distorts the short-circuit current) and/or shunt resistance (which primarily affects the open-circuit voltage).

The Conclusion has been revised according to the Reviewer's advice — see page 17, 1st and 2nd paragraph

The feasibility of using relative changes in short-circuit current, open-circuit voltage, fill factor, and efficiency resulting from the dissociation of FeB pairs to estimate the concentration of iron impurities in a solar cell has been analyzed. Two key metrics were used to identify the solar cell parameter whose changes, resulting from the $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ reconstruction, enable the most reliable determination of iron concentration. Specifically, these metrics are: (1) the monotonicity of the relative change in the parameter value as a function of impurity concentration, which is a necessary condition for the unambiguous estimation of N_{Fe}; and (2) the absolute magnitude of the parameter change, which allows for more precise measurements and, consequently, a more accurate estimation of N_{Fe}. The first criterion is not satisfied by εFF, εV_{OC}, and $\varepsilon \eta$ (the latter two under AM1.5 illumination). At the same iron concentration, εI_{SC} values under monochromatic illumination exceed those under AM1.5 illumination. As mentioned earlier, this effect deals with differences in the generation locations of non-equilibrium carriers under different lighting conditions. Additionally, under identical conditions, the changes in open-circuit voltage are significantly weaker than those in short-circuit current or efficiency. Since εI_{SC} and $\varepsilon \eta$ are of the same order, it is advisable to select the more reliable parameter using additional metrics. Notably, short-circuit current determination, unlike efficiency, does not require additional calculations and can be directly extracted from the raw measured I-V curves. Furthermore, εI_{SC} is virtually independent of illumination intensity (whereas $\varepsilon \eta$ exhibits a weak dependence), leading to two key advantages: (a) iron concentration can be determined using an uncalibrated for-intensity monochromatic light source; (b) the influence of shading caused by electrodes, along with the antireflective and passivating layers of the solar cell, is reduced.

Thus, short-circuit current is the most suitable parameter for estimating the concentration of iron impurities, as its changes during the $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ transformation can be effectively utilized. Determining photovoltaic parameters under monochromatic illumination, with a wavelength corresponding to the predominant absorption in the solar cell base, is more effective than using AM1.5 illumination. The most viable alternatives are solar cell efficiency and open-circuit voltage; however, their applicability is limited at low base doping levels ($< 10^{16}$ cm^{-3}) due to non-monotonic variations in response to increasing iron concentration. In our view, using the fill factor for iron concentration estimation is impractical. These conclusions are validated by experimental results, which show that short-circuit current provides the most accurate determination of iron concentration.

Comment 7. *An Author must improve the introduction section in the application part through the recent referencs CuO-La2O3 Composite-Enabled MIS Schottky Barrier Diodes: A Novel Approach to Optoelectronic Device Diversification; Enhancing photovoltaic applications through precipitating agents in ITO/CIS/CeO2/Al heterojunction solar cell; Manifestation on the choice of a suitable combination of MIS for proficient Schottky diodes for optoelectronics applications: A comprehensive review.*

Reply:

We sincerely thank the Reviewer for suggesting the inclusion of recent references (cited as References 2, 3, and 9 in the revised manuscript). Below, we present an improved version of the 1st paragraph of Introduction.

The necessity for renewable energy sources to meet the growing global demand for sustainable and environmentally friendly energy alternatives has become evident. Among the wide range of renewable energy sources, sunlight is the cleanest, safest, and most abundant source for use in sustainable energy to support economic growth [1]. The utilization of solar energy heavily depends on the use of photovoltaic cells. The development of next-generation solar cells is primarily driven by the search for novel materials suitable for their fabrication. Particular attention is given to exploring the potential use of composites and nanoparticles (e.g., Cu-La-based systems [2], cerium oxide, and copper indium sulfate [3]), MAX phases [4,5], and chalcogenides (such as GeSe, MoSe$_2$, Sb$_2$Se$_3$, and SnSe as hole transport materials [6] or SnS$_2$ and WS$_2$ as electron transport materials [7]), as well as metal silicides (e.g., FeSi$_2$ as an absorber layer [8]). These studies cover a broad range of materials [9], with the primary goal of developing highly efficient and cost-effective photovoltaic devices. Frequently, these novel materials are integrated with silicon in solar cells [8,10]. However, it is worth noting that traditional silicon-based devices continue to play a dominant role in the photovoltaic market [11,12].

Response to Reviewer #2

Comment 1. *The abstract section should be more informative.*

Reply:

We revised the abstract to maximize its informativeness while adhering to the 150-word limit imposed by Materials Science and Engineering: B.

Comment 2. *The novelty of the work is missing in the introduction. Authors should explain what are the key advantages of iron's impact on silicon solar cell?*

Reply:

Iron atoms have no beneficial effects on silicon solar cells; instead, they act as detrimental impurities that significantly reduce carrier lifetime. Despite their harmful impact, iron atoms are among the most common impurities in silicon solar cells. Therefore, our study, which examines their effects on solar cell performance under various conditions and lays the foundation for a rapid, non-destructive detection method, holds significant practical value.

The reviewer correctly noted the lack of a clear novelty statement in the Introduction. In the revised manuscript, we have included the relevant information to address this issue — see page 2, last five paragraph.

> Finally, in our calculations, we attempted to use the latest literature data concerning the exact values of silicon parameters, including light absorption values [39] and coefficients characterizing intrinsic recombination [25, 26].
> The contributions of this work are as follows:
> - The impact of FeB pair dissociation on the short-circuit current, open-circuit voltage, fill factor, and efficiency of silicon solar cells was investigated through simulation. Calculations were performed over various temperatures, illumination conditions, and solar cell parameters, including base thickness, doping level, and impurity concentration. Particular attention was given to the silicon and defect parameters value under diverse conditions.
> - A series of experiments have been done to check the simulation predictions.
> - The feasibility of using variations in short-circuit current, open-circuit voltage, fill factor, and efficiency due to impurity pair dissociation for iron concentration estimation was analyzed, and the most reliable parameter — short-circuit current under monochromatic illumination — was identified.
> - The potential of simultaneous using multiple photovoltaic parameters for iron quantification, including machine learning techniques, was explored. It was shown that applying Principal Component Analysis as a preprocessing step is beneficial in this case.

Comment 3. *Authors should improve the image quality of all figures.*

Reply:

Comment 4. *Author should explain how does the band alignment affect the overall performance of the solar cell?*

Reply:

Band alignment plays a crucial role in determining the efficiency and overall performance of a solar cell. It affects charge carrier separation, transport, and recombination, which directly impact power conversion efficiency. The relative positions of the conduction and valence bands across the junction establish the built-in potential. An optimal band alignment ensures that the built-in field is sufficiently strong to separate photogenerated electron–hole pairs effectively. The conduction band offset and valence band offset determine the energy barriers for minority and majority carrier injection. A too-large offset may impede carrier transport (lowering short-circuit current) or increase the dark current, adversely affecting the open-circuit voltage and fill factor. Proper band alignment between silicon and contact materials (such as metal electrodes or passivation layers) ensures efficient extraction of electrons and holes. Poor alignment can lead to high surface recombination, limit open-circuit voltage and overall efficiency. If the conduction or valence bands are too sharply misaligned, tunneling effects or interface defects may occur, leading to undesirable leakage currents.

Simultaneously, it is essential to emphasize that defect reconstruction $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$, which was the central focus of our work, does not affect band alignment. Although the doping level of the solar cell's base and band alignment are interrelated, and thus, band alignment influences changes in photoelectric conversion parameters resulting from the reconstruction of iron-related defects However, our study did not aim to explore these effects. Instead, we examined the correlations between parameter changes and defect concentration, doping level, base thickness, and temperature.

Comment 5. *What are the primary sources of iron contamination in silicon used for solar cells?*
Reply:

Contaminants can be classified as either grown-in (resulting from impurities in polysilicon feedstock or contamination during crystal growth) or introduced from various sources, such as chemicals (e.g., gases, wet chemistry, photoresist, water), processing equipment (e.g., furnaces, ion implanters, reactive ion etching and rapid thermal annealing systems, polishing machines, electrical measurement tools, wafer handlers, and tools for numbering or marking), and handling between processing steps (e.g., wafer carriers or even ambient air) [40].

Our study focused on monocrystalline silicon solar cells. Notably, iron concentration in crystals grown using either the Czochralski or float-zone method is generally low, with the primary sources of iron contamination being external. However, iron is one of the most abundant elements in nature and is difficult to eliminate in a production environment. Stainless steel, widely used in fabrication facilities, is considered one of the major sources of iron contamination. During manufacturing, numerous opportunities exist for iron to transfer from the production line onto the surface of silicon wafers, from where it can diffuse into the bulk during subsequent thermal processes [40, 41].

The main sources of iron contamination include [40, 41]:
- Cleaning processes (due to residual impurities in chemicals);
- Annealing and oxidation (from furnaces in general and heating coils in particular);
- Equipment utilizing plasma and ions (e.g., ion implantation, dry etching, resist ashing, sputtering, plasma CVD equipment);
- Wafer handling and transportation, despite the widespread use of plastic rather than metal components.

For example, in the samples used in our experimental tests to verify the simulation results, iron contamination primarily originates from chemicals that are not sufficiently pure.

The information about the primary sources of iron contamination in silicon used for solar cells has been added to the revised manuscript — see page 1, 1st paragraph from the bottom

> Iron is prominent among metallic contaminants, with its atoms being among the most prevalent and detrimental impurities in silicon solar cells (SSCs) [42]. The main sources of iron contamination in monocrystalline SSCs include [40, 41] cleaning processes (due to residual impurities in chemicals), annealing and oxidation (from furnaces in general and heating coils in particular), equipment utilizing plasma and ions (e.g., ion implantation, dry etching, resist ashing, sputtering), wafer handling and transportation(despite the widespread use of plastic rather than metal components). Even in small concentrations (about 10^{10} cm^{-3}), point defects related to Fe can significantly influence the performance of SSCs [43, 44]. Therefore, it is of critical importance to assess the concentration of iron impurities. In response to this challenge, various methodologies have been put forward, often based on the property of iron atoms to form pairs with acceptors.

Comment 6. *What role do recombination centers created by iron play in the modeling of solar cell performance?*
Reply:

Iron-related defects are a primary cause of charge carrier recombination. In our simulations using the SCAPS-1D software, we accounted for these defects by incorporating specific parameters, including defect energy levels, electron and hole capture cross-sections, and defect concentrations. The recombination processes were modeled using the Shockley-Read-Hall formalism. A detailed description of the simulation process is provided in Section 2.1. Overall, the presence of recombination centers associated with iron leads to decreases in minority carrier lifetime, short-circuit current, open-circuit voltage, solar cell efficiency, and fill factor.

Comment 7. *Author should discuss and cited recent Si based solar cell in the revised manuscript: DOI : 10.1016/j.mseb.2024.117360, DOI : 10.1016/j.mseb.2023.117141, DOI : 10.1016/j.mseb.2024.117817, DOI : 10.1007/s42247 − 024 − 00821 − y, DOI : 10.1016/j.inoche.2024.112785*
Reply:

We sincerely appreciate the reviewer's valuable suggestion. Most of the recommended works are highly relevant, and we have cited them in multiple sections of the manuscript. Advised articles are referenced as References 8, 4, 6, 7, and 5 in the revised version.

So, we discuss and cited suggested papers in the Introduction, first paragraph

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The necessity for renewable energy sources to meet the growing global demand for sustainable and environmentally friendly energy alternatives has become evident. Among the wide range of renewable energy sources, sunlight is the cleanest, safest, and most abundant source for use in sustainable energy to support economic growth [1]. The utilization of solar energy heavily depends on the use of photovoltaic cells. The development of next-generation solar cells is primarily driven by the search for novel materials suitable for their fabrication. Particular attention is given to exploring the potential use of composites and nanoparticles (e.g., Cu-La-based systems [2], cerium oxide, and copper indium sulfate [3]), MAX phases [4,5], and chalcogenides (such as GeSe, $MoSe_2$, Sb_2Se_3, and SnSe as hole transport materials [6] or SnS_2 and WS_2 as electron transport materials [7]), as well as metal silicides (e.g., $FeSi_2$ as an absorber layer [8])

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Despite its one-dimensional modeling approach, SCAPS is extensively used for modeling various types of solar cells [6,7,8,Joshi2024,Ravidas2024,Liu2024,You2023] in general and for investigating the effects of defects on their performance [6,8,AitAbdelkadir2023,Liang2024,SCAPSDefect3] in particular.

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Impact of change of iron defects was investigated as a function of temperature from 290 K to 340 K, base depth from 180 μm to 380 μm, base doping level from 10^{15} cm^{-3} to 10^{17} cm^{-3}, and total impurity iron atom concentration from 10^{10} cm^{-3} to 10^{14} cm^{-3}. It is worth noting that investigating the effects of doping density, defect density, temperature, and active layer thickness on photovoltaic parameters is a well-established practice [6,7,8]. For each illumination scenario, calculations were carried out with 11 different temperature values and 5 base depth values, evenly distributed within the specified ranges.

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However, the effect of N_B via D_n and L_n is significantly weaker than its influence through E_F and SCR depth variations. Minor effects are expected as well due to both bandgap narrowing and changes in light absorption by free carriers with varying doping levels. The impact of doping level on photovoltaic parameters has been studied in heterojunction [8], thin-film [10], and perovskite [6] solar cells. Moreover, it has been shown [10] that doping concentration variations affect other barrier structure parameters, such as saturation current and ideality factor.

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- At low boron concentrations ($N_B < 10^{16}$ cm^{-3}), the dependence of εFF on N_{Fe} is notably non-linear. Within the used concentration range, two regions of decrease and two regions of increase in εFF are observed. A similar relationship between the fill factor and defect concentration was observed in $BaZrSe_3$–based perovskite solar cells [6];

Comment 8. *How does the modeling in this study contribute to the design of processes for impurity control in silicon?*
Reply:

Comment 9. *State the main findings in the conclusions.*
Reply:

References

[1] A. A. Istratov, H. Hieslmair, E. Weber, Iron and its complexes in silicon, Appl. Phys. A: Mater. Sci. Process. 69 (1999) 13–44.

[2] K. Gwozdz, V. Kolkovsky, Fe-related defects in si: Laplace deep-level transient spectroscopy studies, Phys. Status Solidi A 219 (2022) 2200139.

[3] I. Jyothi, V. Janardhanam, H. Hong, C.-J. Choi, Current–voltage and capacitance–voltage characteristics of al schottky contacts to strained si-on-insulator in the wide temperature range, Mater. Sci. Semicond. Process. 39 (2015) 390–399.

[4] L. Kimerling, J. Benton, Electronically controlled reactions of interstitial iron in silicon, Physica B+C 116 (1983) 297–300.

[5] C. K. Tang, L. Vines, V. P. Markevich, B. G. Svensson, E. V. Monakhov, Divacancy-iron complexes in silicon, J. Appl. Phys. 113 (2013) 044503.

[6] G. Zoth, W. Bergholz, A fast, preparation-free method to detect iron in silicon, J. Appl. Phys. 67 (1990) 6764–6771.

[7] 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.

[8] O. Olikh, V. Kostylyov, V. Vlasiuk, R. Korkishko, Y. Olikh, R. Chupryna, Features of FeB pair light-induced dissociation and repair in silicon n+-p-p+ structures under ultrasound loading, J. Appl. Phys. 130 (2021) 235703.

[9] T. Mchedlidze, L. Scheffler, J. Weber, M. Herms, J. Neusel, V. Osinniy, C. Moller, K. Lauer, Local detection of deep carrier traps in the pn-junction of silicon solar cells, Appl. Phys. Lett. 103 (2013) 013901.

[10] J. Schön, H. Habenicht, M. C. Schubert, W. Warta, Understanding the distribution of iron in multicrystalline silicon after emitter formation: Theoretical model and experiments, J. Appl. Phys. 109 (2011) 063717.

[11] V. Vähänissi, A. Haarahiltunen, H. Talvitie, M. Yli-Koski, H. Savin, Impact of phosphorus gettering parameters and initial iron level on silicon solar cell properties, Progress in Photovoltaics: Research and Applications 21 (2013) 1127–1135.

[12] V. Vähänissi, H. S. Laine, Z. Liu, M. Yli-Koski, A. Haarahiltunen, H. Savin, Full recovery of red zone in p-type high-performance multicrystalline silicon, Sol. Energ. Mat. Sol. 173 (2017) 120–127.

[13] T. Mchedlidze, C. Möller, K. Lauer, J. Weber, Evolution of iron-containing defects during processing of si solar cells, J. Appl. Phys. 116 (2014) 245701.

[14] 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.

[15] 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.

[16] J. Tan, D. Macdonald, F. Rougieux, A. Cuevas, Accurate measurement of the formation rate of iron–boron pairs in silicon, Semicond Sci. Technol. 26 (2011) 055019.

[17] S. Yamaguchi, B. B. Van Aken, A. Masuda, K. Ohdaira, Potential-induced degradation in high-efficiency n-type crystalline-silicon photovoltaic modules: A literature review, Sol. RRL 5 (2021) 2100708.

[18] R. Pässler, Dispersion-related description of temperature dependencies of band gaps in semiconductors, Phys. Rev. B 66 (2002) 085201.

[19] D. Yan, A. Cuevas, Empirical determination of the energy band gap narrowing in p$^+$ silicon heavily doped with boron, J. Appl. Phys. 116 (2014) 194505.

[20] R. Couderc, M. Amara, M. Lemiti, Reassessment of the intrinsic carrier density temperature dependence in crystalline silicon, J. Appl. Phys. 115 (2014) 093705.

[21] M. A. Green, Intrinsic concentration, effective densities of states, and effective mass in silicon, J. Appl. Phys. 67 (1990) 2944–2954.

[22] W. O'Mara, R. Herring, L. Hant, Handbook of semiconductor silicon technology, Noyes Publications, New Jersey, USA, 1990.

[23] D. Klaassen, A unified mobility model for device simulation — I. model equations and concentration dependence, Solid-State Electron. 35 (1992) 953– 959.

[24] A. Fell, K. R. McIntosh, P. P. Altermatt, G. J. M. Janssen, R. Stangl, A. Ho-Baillie, H. Steinkemper, J. Greulich, M. Müller, B. Min, K. C. Fong, M. Hermle, I. G. Romijn, M. D. Abbott, Input parameters for the simulation of silicon solar cells in 2014, IEEE J. Photovolt. 5 (2015) 1250–1263.

[25] T. Niewelt, B. Steinhauser, A. Richter, B. Veith-Wolf, A. Fell, B. Hammann, N. Grant, L. Black, J. Tan, A. Youssef, J. Murphy, J. Schmidt, M. Schubert, S. Glunz, Reassessment of the intrinsic bulk recombination in crystalline silicon, Sol. Energ. Mat. Sol. 235 (2022) 111467.

[26] L. E. Black, D. H. Macdonald, On the quantification of Auger recombination in crystalline silicon, Sol. Energ. Mat. Sol. 234 (2022) 111428.

[27] P. P. Altermatt, J. Schmidt, G. Heiser, A. G. Aberle, Assessment and parameterisation of Coulomb–enhanced Auger recombination coefficients in lowly injected crystalline silicon, J. Appl. Phys. 82 (1997) 4938–4944.

[28] W. Wijaranakula, The reaction kinetics of iron–boron pair formation and dissociation in p–type silicon, J. Electrochem. Soc. 140 (1993) 275–281.

[29] J. D. Murphy, K. Bothe, M. Olmo, V. V. Voronkov, R. J. Falster, The effect of oxide precipitates on minority carrier lifetime in p–type silicon, J. Appl. Phys. 110 (2011) 053713.

[30] O. Olikh, O. Lozitsky, O. Zavhorodnii, Estimation for iron contamination in si solar cell by ideality factor: Deep neural network approach, Prog. Photovoltaics Res. Appl. 30 (2022) 648–660.

[31] O. Olikh, Relationship between the ideality factor and the iron concentration in silicon solar cells, Superlattices Microstruct. 136 (2019) 106309.

[32] 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.

[33] F. E. Rougieux, C. Sun, D. Macdonald, Determining the charge states and capture mechanisms of defects in silicon through accurate recombination analyses: A review, Sol. Energy Mater. Sol. Cells 187 (2018) 263 – 272.

[34] B. B. Paudyal, K. R. McIntosh, D. H. Macdonald, Temperature dependent electron and hole capture cross sections of iron-contaminated boron-doped silicon, in: 2009 34th IEEE Photovoltaic Specialists Conference (PVSC), pp. 001588–001593.

[35] 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.

[36] B. Sultana, M. Ferdous Rahman, A. Chandra Roy, M. Masum Mia, M. Al Ijajul Islam, A. Irfan, A. Rasool Chaudhry, M. Dulal Haque, A novel design and optimization of si based high performance double absorber heterojunction solar cell, Materials Science and Engineering: B 304 (2024) 117360.

[37] T. Akila, P. Gayathri, G. Alan Sibu, V. Balasubramani, H. Al-Lohedan, D. M. Al-Dhayan, Augmented photovoltaic performance of cu/ce-(sn:cd)/n-si schottky barrier diode utilizing dual-doped ce-(sn:cd) thin films, Opt. Mater. 149 (2024) 115133.

[38] M. Masum Mia, M. Faruk Hossain, M. Rahman, N. Badi, A. Irfan, M. Ferdous Rahman, Unveiling the impact of se based htm on bazrse3 perovskites solar cell and improving the theoretical efficiency above 32%, Materials Science and Engineering: B 311 (2025) 117817.

[39] M. A. Green, Improved silicon optical parameters at 25°C, 295 K and 300 K including temperature coefficients, Prog. Photovoltaics Res. Appl. 30 (2022) 164–179.

[40] A. A. Istratov, H. Hieslmair, E. Weber, Iron contamination in silicon technology, Appl. Phys. A 70 (2000) 489–534.

[41] M. D. Abbott, D. Poplavskyy, G. Scardera, D. Inns, F. Lemmi, K. R. McIntosh, S. C. Baker-Finch, Iron contamination in silicon solar cell production environments, in: 2014 IEEE 40th Photovoltaic Specialist Conference (PVSC), pp. 3479–3484.

[42] T. Buonassisi, A. A. Istratov, M. D. Pickett, M. Heuer, J. P. Kalejs, G. Hahn, M. A. Marcus, B. Lai, Z. Cai, S. M. Heald, Chemical natures and distributions of metal impurities in multicrystalline silicon materials, Prog. Photovolt.: Res. Appl. 14 (2006) 513–531.

[43] M. Schubert, M. Padilla, B. Michl, L. Mundt, J. Giesecke, J. Hohl-Ebinger, J. Benick, W. Warta, M. Tajima, A. Ogura, Iron related solar cell instability: Imaging analysis and impact on cell performance, Sol. Energy Mater. Sol. Cells 138 (2015) 96–101.

[44] A. Herguth, Quantification of iron in boron-doped silicon solar cells from open circuit voltage measurements, IEEE J. Photovolt. 12 (2022) 937–947.