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Iron's impact on silicon solar cell execution: comprehensive modeling across diverse scenarios
--Manuscript Draft--

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Abstract:	Silicon solar cells are vital for renewable energy but often degrade from iron-induced carrier recombination. This study investigates the impact of iron-related defect variability on the photovoltaic performance of n+-p-p+ structure through comprehensive SCAPS simulations and experimental measurements. The effect of iron-boron pair dissociation on silicon solar cell (SSC) short-circuit current, open-circuit voltage, fill factor, and efficiency was analyzed under diverse conditions. Simulations covered temperatures (290–340 K), iron concentrations (10 ¹⁰ -10 ¹⁴ cm ⁻³), and SSC base thicknesses (180-380 μm) and boron doping (10 ¹⁵ -10 ¹⁷ cm ⁻³) under AM1.5 and monochromatic (940 nm) illumination. Experimental results confirmed simulation predictions. The study assessed the ability to use photovoltaic parameter variations for iron quantification, identifying short-circuit current under monochromatic light as a highly reliable metric. The study correlations between photovoltaic characteristics suggested that Principal Component Analysis is advisable for dimensionality reduction when SSC multiple parameters are used in non-invasive iron detection.

To: Materials Science and Engineering: B Editorial Board
Subject: Article Submit

Dear Editors,

Enclosed with this letter you will find the electronic submission of manuscript entitled “Iron’s impact on silicon solar cell execution: comprehensive modeling across diverse scenarios” by Oleg Olikh and Oleksii Zavhorodnii.

It is widely recognized that defects can significantly alter the properties of semiconductors, and understanding the mechanisms behind these alterations is essential for optimizing solar cell efficiency. Over the years, researchers have accumulated considerable knowledge about various defects. Our investigation aims to examine the impact of iron-related defect variability on the performance of silicon-based solar cells, integrating both modeling and experimental validation.

Our research reveals that changes in short-circuit current provide the most reliable method for estimating iron impurity concentrations, significantly improving over traditional techniques. We also found that the behavior of open-circuit voltage is non-monotonic at low boron doping levels, indicating a complex interaction between doping and defect dynamics. We believe that our research not only enhances the understanding of iron-related defects but also has practical implications for developing methods to characterize impurity concentration in silicon solar cells from current-voltage characteristic. Such approach involves quantifying photovoltaic energy conversion parameters (short-circuit current, open-circuit voltage, solar cell efficiency, fill factor) and then employing these values as input features for machine learning models. One of the finding of this research is the expedience of principal component analysis in this context. Given the growing interest in renewable energy technologies and machine learning, we are confident that our findings will resonate with your readership and stimulate further exploration in this area.

This is an original paper which has not been simultaneously submitted as a whole or in part anywhere else. No elements of the work have been published in any form. No conflict of interest exists in the submission of this manuscript.

We would very much appreciate if you would consider the manuscript for publication in the *Materials Science and Engineering: B*.

Sincerely yours,
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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 photovoltaic parameters (PVPs) is due to Fe_{*i*}B_{Si} pairs and Fe_{*i*} is fully justified. Furthermore, we emphasize that this paper focuses on the relative changes in parameters during Fe_{*i*}B_{Si} ⇌ 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]:

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

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 6, 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 [29,74]. 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 paragraph), page 4 (1st and 2nd 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 [53];
- doping induced bandgap narrowing according to Yan & Cuevas [54];
- effective density of states at conduction and valence band and intrinsic carrier concentration according to Couderc et al. [55];
- thermal carrier velocities according to Green [56];
- free carrier effective masses according to O'Mara et al. [57];
- carrier mobilities according to Klaassen's theory [58];

The values of surface recombination coefficients were considered equal to the thermal velocities of carriers [44]. 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.[42]) and Auger recombination (where the coefficients considered the effect of Coulomb enhancement [43] and temperature dependence [59]).

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

Case 2. Iron atoms predominantly form pairs with acceptors, $[Fe_iB_s] \gg [Fe_i]$, but the exact concentration ratio depends on the position of the Fermi level and temperature [60,61] 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 [38,37]. This case corresponds to prolonged storage of the structure in darkness or under conditions of low-intensity ($< 0.01 \text{ J cm}^{-2}$ [40]) 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 [62,63,64].

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: $(T, d_p, N_B, \epsilon I_{SC})$. Evidently, incorporating additional information, such as changes in efficiency ($\epsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta)$, 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 $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_B, \epsilon I_{SC})$. 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 $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}, \epsilon FF)$ 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 PVPs. 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 14, 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 $(T, d_p, N_B, \epsilon I_{SC})$. Evidently, incorporating additional information, such as changes in efficiency ($\epsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta)$, 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 ϵI_{SC} and $\epsilon\eta$ 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 $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_B, \epsilon I_{SC})$.

and on page 16, 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 [83]. 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 PVPs 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 $(T, d_p, N_B, \epsilon I_{SC})$, 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 $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}, \epsilon FF)$ 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 PVPs, it is advisable to apply PCA to transform the original data. Thus, the simultaneous use of $\epsilon\eta$ 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 PVP values 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 [18, 19]. 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 PVPs 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 [20], 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 PVPs has been studied in heterojunction [21], thin-film [22], and perovskite [23] solar cells. Moreover, it has been shown [22] 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 8, paragraph 1. Reference is included in the revised manuscript (references 10)

...while the presence of the acceptor state Fe_iB_s causes the carrier lifetime to be doping-dependent under low injection conditions [39].

The relationship between N_{B} and E_{F} is the key factor in the influence of doping level on the sensitivity of PVPs to iron presence. Specifically, the rate of SRH recombination — and consequently, variations in PVPs 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 [60,61]. 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 PVPs 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 [58], 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 PVPs 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 $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$ 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 , $\varepsilon V_{\text{OC}}$, and $\varepsilon \eta$ (the latter two under AM1.5 illumination). At the same iron concentration, $\varepsilon I_{\text{SC}}$ 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 $\varepsilon I_{\text{SC}}$ 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, $\varepsilon I_{\text{SC}}$ 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 $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$ transformation can be effectively utilized. Determining PVPs 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 ($< 10^{16} \text{ cm}^{-3}$) 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 text has been revised according to the Reviewer's advice — see page 14, 2nd paragraph from the bottom

The revealed characteristics of $\varepsilon\eta$ indicate that this PVP is entirely suitable for estimating iron concentration.

Two key metrics were used to identify the solar cell parameter whose changes, resulting from the $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$ 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 , $\varepsilon V_{\text{OC}}$, and $\varepsilon\eta$ (the latter two under AM1.5 illumination). At the same iron concentration, $\varepsilon I_{\text{SC}}$ 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 $\varepsilon I_{\text{SC}}$ 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, $\varepsilon I_{\text{SC}}$ 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.

Comment 7. An Author must improve the introduction section in the application part through the recent references *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, MoSe₂, Sb₂Se₃, and SnSe as hole transport materials [6] or SnS₂ and WS₂ as electron transport materials [7]), as well as metal silicides (e.g., FeSi₂ 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 [41] and coefficients characterizing intrinsic recombination [42,43].

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 PVPs 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:

We have modified Figs. 1, 2, 4, 5, 7, 9, 11, and 12 to improve clarity and readability. The captions of Figs. 1, 2, 4, 5, 7, and 11 have been revised to enhance interpretability. To improve quality, all figures have been recreated in higher resolution.

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 $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$, 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 photovoltaic 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) [24].

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 [24, 25].

The main sources of iron contamination include [24, 25]:

- 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) [24]. The main sources of iron contamination in monocrystalline SSCs include [17,25] 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 [26,27]. 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

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, MoSe₂, Sb₂Se₃, and SnSe as hole transport materials [6] or SnS₂ and WS₂ as electron transport materials [7]), as well as metal silicides (e.g., FeSi₂ as an absorber layer [8])

on page 3, second paragraph in Section 2.1

Despite its one-dimensional modeling approach, SCAPS is extensively used for modeling various types of solar cells [6,7,8,46,47,48,49] in general and for investigating the effects of defects on their performance [6,8,50,51,52] in particular.

on page 5, 2nd paragraph

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 PVPs 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.

on page 8, 1st paragraph from the bottom

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 PVPs 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.

on page 12, 5th paragraph from the top

- At low boron concentrations ($N_{\text{B}} < 10^{16} \text{ cm}^{-3}$), 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 BaZrSe₃-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:

Our study lays the groundwork for developing an efficient, express, cost-effective method for monitoring iron impurity concentrations in silicon solar cells. This approach relies on current-voltage measurements and can be easily incorporated into the standard characterization procedure for silicon photovoltaic devices. Through simulations and experiments, we have identified a key metric for quantifying iron impurities (short-circuit current) and determined which factors significantly (base doping level, temperature) and insignificantly (base thickness) influence the response

of solar cells to iron-related defect rearrangements. These findings should be considered when implementing the method in practice. Our approach allows for the simultaneous determination of the concentration of iron impurities along with the standard solar cell parameters (such as short-circuit current, open-circuit voltage, and nominal power), all without needing additional equipment.

Thanks to the Reviewer's comment, we refined one of our study's conclusions, which has been incorporated into the Conclusion section (see last paragraph).

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

Reply:

In response to the Reviewer's comments, we have expanded the Conclusion section and clearly formulated all main findings. Below is the revised version of the Conclusions, with the changes highlighted in red in the updated manuscript.

We have provided the results of modeling the impact of variations in the state of iron impurities on the PVPs of silicon solar cells with different base properties under various external conditions (temperature, intensity, and spectral composition of illumination). The simulation results have been compared with experimental data.

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. It is shown that short-circuit current is the most suitable parameter for iron quantification, as variations in I_{SC} value during the $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$ transformation can be effectively utilized. Determining PVPs 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 ($< 10^{16} \text{ cm}^{-3}$) 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.

It has been shown that the potential accuracy of estimating iron concentration depends on the doping level of the base: at a boron concentration around 10^{16} cm^{-3} , it is minimal, while decreasing or increasing this value enhances the response of I_{SC} to the presence of iron. Furthermore, the accuracy of N_{Fe} determination is significantly influenced by the availability of precise information on the doping level of the base, as well as the accuracy of estimating the intensity of monochromatic illumination, especially when using $\varepsilon\eta$ and $\varepsilon V_{\text{OC}}$.

At the same time, $\varepsilon\eta$ and $\varepsilon V_{\text{OC}}$ can serve as additional parameters for refining the determination of iron concentration. In our opinion, for estimating iron concentration through changes in PVP values due to variability in iron-related defects, it is advisable to use a set of $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$ or $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}}, \varepsilon\eta, \varepsilon V_{\text{OC}})$. Furthermore, it has been demonstrated that iron-induced changes in various PVPs are correlated. Therefore, if iron concentration estimation is performed using changes in multiple PVPs, applying Principal Component Analysis is advisable. This data transformation reduces the number of variables while preserving the maximum variance information and accelerating calculations.

Our study lays the groundwork for developing an efficient, express, cost-effective method for monitoring iron impurity concentrations in silicon solar cells. This approach relies on current-voltage measurements and can be easily incorporated into the standard characterization procedure for silicon photovoltaic devices. Through simulations and experiments, we have identified a key metric for quantifying iron impurities (short-circuit current) and determined which factors significantly (base doping level, temperature) and insignificantly (base thickness) influence the response of solar cells to iron-related defect rearrangements. These findings should be considered when implementing the method in practice. Our approach allows for the simultaneous determination of the concentration of iron impurities along with the standard solar cell parameters (such as short-circuit current, open-circuit voltage, and nominal power), all without needing additional equipment. The suggested and verified approach advances our understanding of impurity effects and paves the way for improved solar cell reliability.

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Highlights

Iron's impact on silicon solar cell execution: comprehensive modeling across diverse scenarios

Oleg Olikh,Oleksii Zavhorodnii

- Iron defect transformation impact on Si solar cells was studied via SCAPS simulation
- Variations in I_{SC} , V_{OC} , and η due to FeB decay allow estimation of iron contamination
- Short-circuit current variation is a key iron impurity quantification metric
- PCA is advisable step for estimating iron concentration using photovoltaic parameters

Iron's impact on silicon solar cell execution: comprehensive modeling across diverse scenarios

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ABSTRACT

Silicon solar cells are vital for renewable energy but often degrade from iron-induced carrier recombination. This study investigates the impact of iron-related defect variability on the photovoltaic performance of $n^+‐p^+$ structure through comprehensive SCAPS simulations and experimental measurements. The effect of iron–boron pair dissociation on silicon solar cell (SSC) short-circuit current, open-circuit voltage, fill factor, and efficiency was analyzed under diverse conditions. Simulations covered temperatures (290–340 K), iron concentrations (10^{10} – 10^{14} cm^{-3}), and SSC base thicknesses (180–380 μm) and boron doping (10^{15} – 10^{17} cm^{-3}) under AM1.5 and monochromatic (940 nm) illumination. Experimental results confirmed simulation predictions. The study assessed the ability to use photovoltaic parameter variations for iron quantification, identifying short-circuit current under monochromatic light as a highly reliable metric. The study correlations between photovoltaic characteristics suggested that Principal Component Analysis is advisable for dimensionality reduction when SSC multiple parameters are used in non-invasive iron detection.

1. 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, MoSe₂, Sb₂Se₃, and SnSe as hole transport materials [6] or SnS₂ and WS₂ as electron transport materials [7]), as well as metal silicides (e.g., FeSi₂ 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].

The issue of semiconductor purity has become increasingly significant since the advent of the transistor in 1947 [13]. The 1960 study by Shockley and Queisser [14] demonstrated that the electrical properties of $n^+‐p$ silicon diodes deteriorate when impurity atoms of metals such as Cu, Fe, Mn, Au, Zn, and Ni are present. As a result, investigations were initiated to prevent metal contamination in semiconductors during manufacturing. In particular, metallic impurities are known to reduce the efficiency of silicon-based devices through direct shunting [15], increased leakage current [16], or bulk recombination [17]. Despite extensive study of metallic impurities in silicon over the past fifty years [13, 18], the problem continues to attract significant attention [19, 20, 21, 22, 23].

Iron is prominent among metallic contaminants, with its atoms being among the most prevalent and detrimental impurities in silicon solar cells (SSCs) [24]. The main sources of iron contamination in monocrystalline SSCs include [17, 25] 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 [26, 27]. Therefore, it is of critical importance to assess the concentration of iron impurities. In response to

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this challenge, various methodologies have been put forward, often based on the property of iron atoms to form pairs with acceptors. In particular, iron atoms are predominantly located in interstitial positions in silicon, forming the Fe_i defect. In *p*-type crystals, without external illumination, iron atoms carry positive charges and tend to bond with negatively charged doping atoms (boron, aluminum, gallium, or indium), forming $\text{Fe}_i\text{B}_{\text{Si}}$ pairs [28]. However, these pairs can destabilize by intense illumination, electron injection, or heating up to 200 °C [29]. The recombination properties of iron-related defects Fe_i and Fe_iB_s differ significantly, which profoundly affects the overall characteristics of the crystal. This fact formed the basis for the first method of assessing iron concentration [30], which relied on measuring the diffusion length of minority carriers using the surface photovoltage method [31]. Many other methods involve measurements of carrier lifetime [32, 33], Quasi-Steady-State Photoconductance [34], or the study of kinetic dependencies of short-circuit current [35] or photoluminescence intensity [36] during the reaction $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$.

Notably, the presence of Fe-related defects affects the dynamics of electron and hole movement within the solar cell, which is reflected in changes to the appearance of the current–voltage (*I*–*V*) characteristics of SSCs overall, as well as modifications to the main photovoltaic parameters (PVPs) (short-circuit current I_{SC} , open-circuit voltage V_{OC} , efficiency η , and fill factor FF) in particular. These findings create fundamental possibilities to advance methods for estimating iron concentration by *I*–*V* curves measuring before and after pair dissolution. The advantages of such an approach are associated with the possibility of directly characterizing finished solar cells, as well as the absence of the need for additional equipment other than that required for *I*–*V* measurements, which is extremely common. Efforts have been made initially in developing such methods. For instance, it was proposed to estimate the concentration of iron in SSCs based on changes in the ideality factor [37, 38] or open-circuit voltage [27]. However, developing such approaches requires evaluating how a particular parameter changes when iron-containing pairs dissolve and determining whether it can estimate the iron concentration N_{Fe} . For example, the most evident conditions for utilizing a specific parameter include its change due to the transformation $\text{Fe}_i\text{B}_{\text{Si}} \rightarrow \text{Fe}_i + \text{B}_{\text{Si}}$, at least by 10 %, along with a monotonic dependence of these changes on N_{Fe} .

This paper intends to determine the variations of I_{SC} , V_{OC} , η , and FF resulting from the decay of iron-containing pairs in boron-doped silicon solar cells. Previous similar calculations have been conducted [39, 26, 19], but the results presented typically pertain only to certain temperatures, illumination levels (often AM1.5), and solar cells with specific parameters. In this study, we performed calculations over a sufficiently wide temperature range (290–340 K) and for solar cells with varying base thickness (180–380 μm) and doping levels (boron concentration in the base ranging from 10^{15} to 10^{17} cm^{−3}). The obtained results enable us to evaluate the feasibility and potential of using the main PVPs of silicon solar cells to estimate the N_{Fe} value across a temperature range close to operating conditions. Furthermore, investigations have explored changes in photovoltaic performance under not only solar illumination (AM1.5G) but also low-intensity monochromatic light (wavelength of 940 nm, intensities of 5 W/m² and 10 W/m²). In the first case, while it is customary to adhere to standard conditions, it's essential to consider that illumination at 1000 W/m² can lead to the decay of Fe_iB_s complexes [40]. Therefore, measurements for cases requiring the presence of undissociated pairs in silicon must meet specific constraints. On the other hand, intentionally chosen monochromatic illumination penetrates the emitter with negligible losses and does not reach the rear side. In this context, the PVPs show remarkable sensitivity to recombination processes occurring within the solar cell base and to iron concentration in this region. Finally, in our calculations, we attempted to use the latest literature data concerning the exact values of silicon parameters, including light absorption values [41] and coefficients characterizing intrinsic recombination [42, 43].

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.

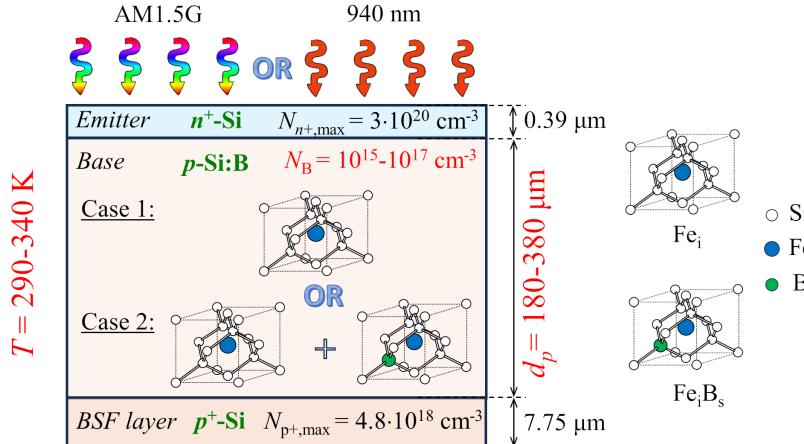


Figure 1: Schematic diagram of analysed solar cell. The figure also presents the solar cell parameters and external conditions that varied during the simulation — see the main text for details. The right side of the figure illustrates the configurations of interstitial iron Fe_i and iron-boron pairs Fe_iB_s .

Table 1

Parameters varied during the simulation

Parameter	Range of values
$d_p (\mu\text{m})$	180 – 380
$N_B (\text{cm}^{-3})$	$10^{15} – 10^{17}$
$N_{\text{Fe}} (\text{cm}^{-3})$	$10^{10} – 10^{14}$
$T (\text{K})$	290 – 340
Illumination	AM1.5G, 1000 W/m ² ; 940 nm, 5 W/m ² ; 940 nm, 10 W/m ²

2. Research Methodology

2.1. Simulation Details

The study involved simulation I - V curves of SSCs with an n^+ - p - p^+ structure, as illustrated in Fig. 1. A back surface field (BSF, p^+ -layer) is a notable feature observed in both Al-BSF cells (full area), which are gradually losing relevance, and PERC cells (locally), which are the most widely used in mass production. The structures with a base uniformly doped with boron were under consideration. The doping concentration N_B , and the base thickness d_p were varied during the modeling process, as detailed in Table 1. The emitter and p^+ -layer were considered to be unevenly doped. The concentration profiles of the dopants, their maximum values ($N_{p^+,\text{max}}$ and $N_{n^+,\text{max}}$), and layer thicknesses (see Fig. 1) were selected according to Fell et al. [44].

The simulation was conducted using the SCAPS 3.3.11 code [45]. SCAPS-1D software, developed by the University of Gent, is founded on theoretical computations that involve solving Poisson's equation, continuity equations for holes and electrons, and drift-diffusion at each position within the solar cell, considering the boundary conditions. Despite its one-dimensional modeling approach, SCAPS is extensively used for modeling various types of solar cells [6, 7, 8, 46, 47, 48, 49] in general and for investigating the effects of defects on their performance [6, 8, 50, 51, 52] in particular.

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 [53];
- doping induced bandgap narrowing according to Yan & Cuevas [54];

- effective density of states at conduction and valence band and intrinsic carrier concentration according to Couderc et al. [55];
- thermal carrier velocities according to Green [56];
- free carrier effective masses according to O'Mara et al. [57];
- carrier mobilities according to Klaassen's theory [58];

The values of surface recombination coefficients were considered equal to the thermal velocities of carriers [44]. 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.[42]) and Auger recombination (where the coefficients considered the effect of Coulomb enhancement [43] and temperature dependence [59]).

When accounting for the influence of iron impurities, we considered that Fe atoms were uniformly distributed within the base and p^+ -layer with a total concentration of N_{Fe} (see Table 1). Two cases were under consideration:

Case 1. The concentration of interstitial iron defects $[\text{Fe}_i] = N_{\text{Fe}}$ at each position throughout the solar cell, with no pairs present $[\text{Fe}_i\text{B}_s] = 0$. This case corresponds to the state of the structure immediately after intense illumination, for example.

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 [60, 61] 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 [38, 37]. This case corresponds to prolonged storage of the structure in darkness or under conditions of low-intensity ($< 0.01 \text{ J cm}^{-2}$ [40]) 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 [62, 63, 64].

As previously mentioned, the solar cell behavior was simulated under different illumination conditions, including solar light (AM1.5G) and monochromatic light (wavelength 940 nm, intensity of $W_{\text{ill}} = 5 \text{ W/m}^2$ or 10 W/m^2) — see Table 1. The calculations incorporated the light absorption values in silicon based on Green's study [41].

The I - V characteristics were simulated for both Case 1 and Case 2 (see Fig. 2), and from each curve, the short-circuit current, open-circuit voltage, efficiency, and fill factor were determined. Assessing the influence of iron defect variability relied on the relative changes in each photovoltaic conversion parameter:

$$\varepsilon A = \frac{A^{\text{FeB}} - A^{\text{Fe}}}{A^{\text{FeB}}} \times 100\%, \quad (1)$$

where A represents one of the parameters (I_{SC} , V_{OC} , η , and FF), superscript "FeB" corresponds to the parameter value for coexistence of Fe_i and Fe_iB_s (Case 2), superscript "Fe" is related to the decay of all pairs (Case 1).

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 PVPs 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. The concentration values were distributed equally on a logarithmic scale with 4 (N_B case) and 6 (N_{Fe} case) steps per decade. As a result, for the AM1.5 illumination scenario, for instance, 24750 I - V characteristics were simulated. An exception occurred with monochromatic illumination at $W_{\text{ill}} = 10 \text{ W/m}^2$, where we used only two d_p values.

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 [63, 65, 66]. 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

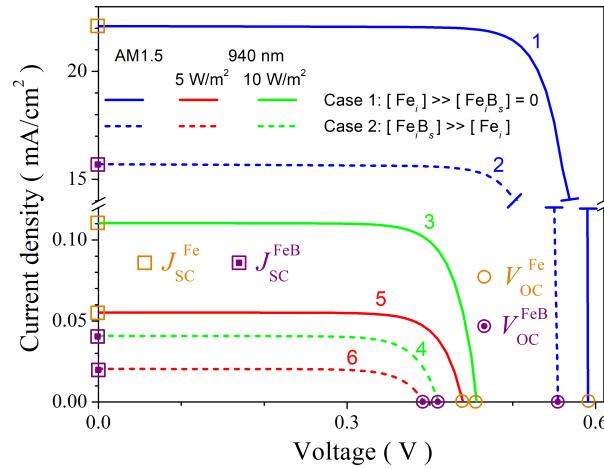


Figure 2: Typical IV characteristics, calculated for structure with $d_p = 180 \mu\text{m}$, $N_B = 10^{17} \text{ cm}^{-3}$, $N_{\text{Fe}} = 10^{14} \text{ cm}^{-3}$ at $T = 290 \text{ K}$. Illumination: AM1.5 (curves 1, 2), 940 nm 10 W/m² (3, 4) and 940 nm 5 W/m² (5, 6). Solid (1, 3, 5) and dotted (2, 4, 6) lines correspond to Case 1 and Case 2, respectively. The figure also indicates the short-circuit current values (squares) and open-circuit voltage values (circles) for two scenarios: the dissociation of all pairs (empty marks), and the coexistence of Fe_i and Fe_iB_s (marks with a dot inside).

impurity atoms pair with acceptors (e.g., boron in Si:B) [28, 63]. 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 [67]. Further supporting this, several methods used to evaluate the total iron concentration in p -Si rely on breaking the FeB pair [30, 36, 35]. 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 [63, 68] in contrast to other iron-related defects. Notably, iron gettering by oxygen precipitates or structural defects increases carrier lifetime [69, 70]. 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 [69, 70, 71] or the formation of a passivating layer [72] 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 photovoltaic parameters is due to Fe_iB_s pairs and Fe_i is fully justified. Furthermore, we emphasize that this paper focuses on the relative changes in parameters during $\text{Fe}_i\text{B}_s \rightleftharpoons \text{Fe}_i + \text{B}_s$ transformation, which enables the isolation of these specific defects' contributions.

2.2. Experimental Details

To evaluate the validity of the simulated results, we also conducted experimental studies on the effect of changing the state of iron-related defects on the PVPs of silicon solar cells.

The $n^+ \text{-} p \text{-} p^+$ -Si samples were used in the experiment. The structure was fabricated from a 380 μm thick p -type boron-doped Czochralski silicon (100) wafer with doping level $N_B = 1.36 \times 10^{15} \text{ cm}^{-3}$. The n^+ emitter with a sheet resistance of about 20–30 Ω/\square and thickness of 0.7 μm was formed by phosphorus diffusion. The anti-recombination isotype barrier was created by using a p^+ layer (10–20 Ω/\square) formed by boron diffusion. On the front surface, SiO_2 (40 nm) and Si_3N_4 (30 nm) films were formed as antireflective and passivating layers, respectively. The solid and grid Al contacts were formed by magnetron sputtering on the back and front surfaces, respectively.

The I - V characteristics were measured using a Keithley 2450 source meter and low-intensity monochromatic light source (light-emitting diode SN-HPIR940nm-1W with light wavelength 940 nm and intensity of about $W_{\text{ill}} = 5 \text{ W/m}^2$).

For different samples, the iron concentration ranged from 2×10^{11} to $4 \times 10^{13} \text{ cm}^{-3}$. The values of N_{Fe} were determined using a methodology [73, 35], based on fitting the kinetics of short-circuit current. The decay of Fe_iB_s pairs was realized using intensive (7000 W/m^2) halogen lamp illumination.

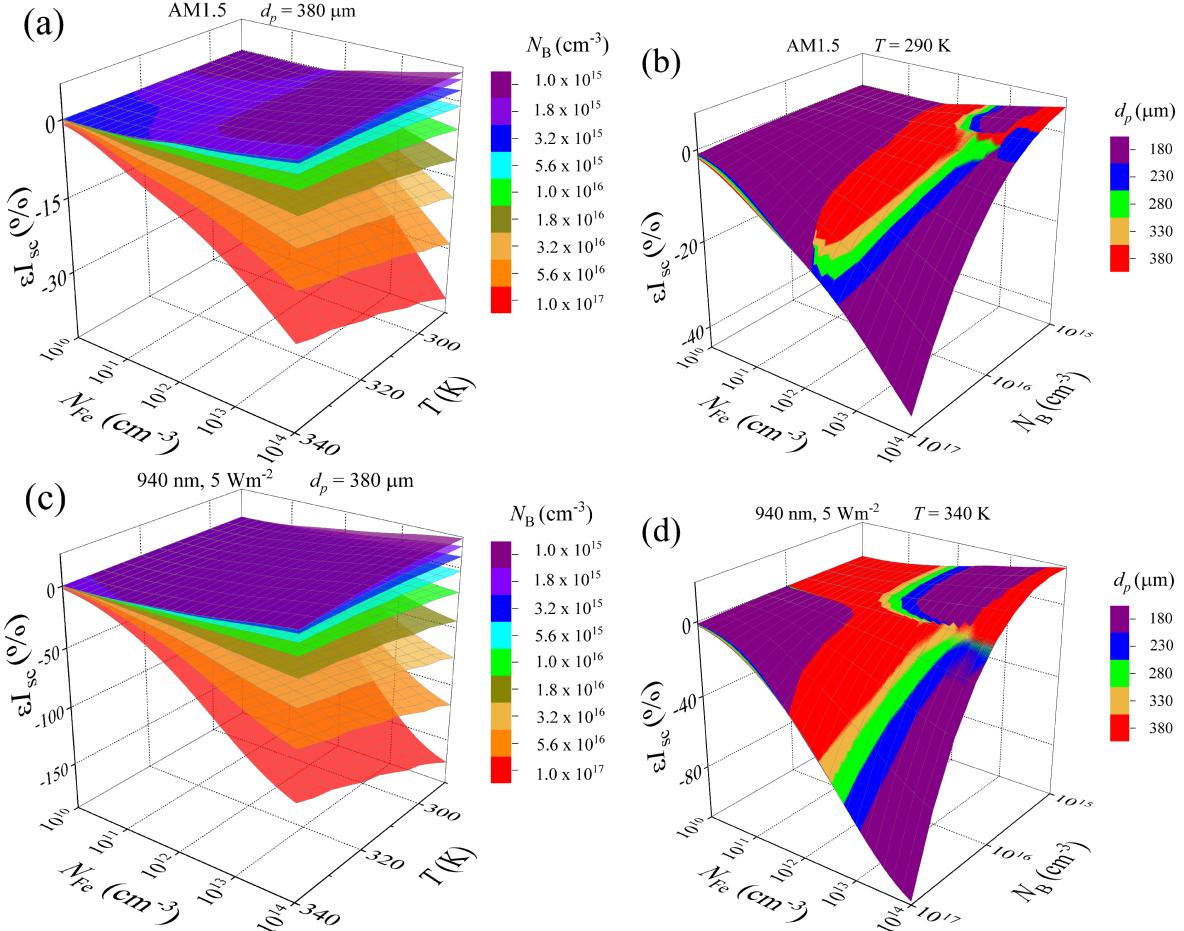


Figure 3: Relative changes in short-circuit current caused by a complete dissociation of Fe_iB_s pairs as a function of iron concentration and temperature (panels a and c) or doping level (b, d). Illumination: AM1.5 (a, b), 940 nm 5 W m^{-2} (c, d). $T, \text{ K}$: 290 (b), 340 (d). Different surfaces correspond to different doping levels (a, c) and base depths (b, d).

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 [29, 74]. These limitations affect the measurement duration at high temperatures, and the experiments accounted for them.

3. Results and Discussion

3.1. Short-circuit current

Figure 3 illustrates the characteristic dependencies of short-circuit current variations resulting from the reconfiguration of iron-containing defects, as obtained from the simulations. We present a more comprehensive set of figures that depict the detailed dependencies of ϵI_{SC} on all parameters varied during the calculations in the Supplementary Material (Figs. S1–S6). It is important to note that the qualitative nature of the short-circuit current variations remains practically identical under both solar and monochromatic illumination, with the quantitative parameters of ϵI_{SC} differing: at 940 nm, the absolute values of ϵI_{SC} are approximately 3–4 times greater than those observed under AM1.5 conditions, assuming other parameters are constant. Among other features of ϵI_{SC} changes, we can highlight the following:

- The module εI_{SC} increases monotonically with increasing iron concentration, but the sign of this value depends on the doping level. At low boron concentrations ($N_B = 10^{15} \text{ cm}^{-3}$) $\varepsilon I_{SC} > 0$, whereas at high concentrations ($N_B = 10^{17} \text{ cm}^{-3}$) $\varepsilon I_{SC} < 0$ — see Figs. 3a, 3c, S3–S6;
- Increasing the acceptor concentration causes a monotonic decrease in εI_{SC} (Figs. 3b, 3d); the N_B value at which the sign of εI_{SC} changes depends on the temperature (decreases with decreasing in T value) and the type of illumination (is generally higher in the case of monochromatic light) — see Fig. S2;
- In the case where $\varepsilon I_{SC} < 0$, an temperature increase causes a decrease in the absolute magnitude of the relative changes in short-circuit current, with the dependence being nearly linear and the slope increasing with higher doping levels and iron concentration (Figs. 3a, 3c, S4). In the case where $\varepsilon I_{SC} > 0$, a T changing results in minor non-monotonic variations of the short-circuit current after the dissociation of Fe_iB_s pairs (Fig. S3);
- The influence of base thickness on εI_{SC} increases with increasing N_B and decreasing N_{Fe} (Figs. S5, S3), but it is minimal overall. As calculations have shown, increasing d_p by more than twice causes changes in εI_{SC} that do not exceed 0.5 %;
- Changing the intensity of the monochromatic illumination (from 5 W/m^2 to 10 W/m^2) does not practically change the value of εI_{SC} ;
- The absolute values of εI_{SC} can reach relatively high values (more than 100 % for 940 nm illumination); however, in cases where $N_{\text{Fe}} < 10^{11} \text{ cm}^{-3}$ and around $N_B = 10^{16} \text{ cm}^{-3}$, the changes in short-circuit current do not exceed a few percent.

The identified features of the εI_{SC} changes can be explained by considering the main reasons for the influence of factors, which varied during simulation, on the photovoltaic conversion. It is known [75] that the main influence of metal impurities on solar cell performance is caused by their effect on the collection efficiency (CE, portion of excess carriers that reach the depletion region of $p-n$ junction). Neglecting the influence of series and shunt resistances, the short-circuit current coincides with the photocurrent I_{ph} , which equals the CE multiplied by the number of light-induced excess carriers. In turn, the CE can be calculated as a convolution of generation function, which is proportional to $\exp(-\alpha z)$ (where α is the absorption coefficient and z is the coordinate along the axis directed perpendicular to the $p-n$ junction from the emitter) and the collection probability, which can be obtained as a solution of homogeneous diffusion equation.

The photogenerated current for the cell can be obtained by adding the relevant quantities for the base $I_{ph,b}$ and the emitter $I_{ph,e}$ [76]:

$$I_{SC} \approx I_{ph} = I_{ph,e} + I_{ph,b}. \quad (2)$$

However, considering the location of the impurity iron, it can be assumed that during the $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$ reconfiguration, the first term on the right-hand side of Eq. (2) remains unchanged ($I_{ph,e}^{\text{FeB}} = I_{ph,e}^{\text{Fe}} = I_{ph,e}$), and therefore, considering Eq. (1):

$$\varepsilon I_{SC} = \frac{I_{ph,b}^{\text{FeB}} - I_{ph,b}^{\text{Fe}}}{I_{ph,e} + I_{ph,b}^{\text{FeB}}} \times 100\%. \quad (3)$$

In turn, the base photocurrent the under monochromatic illumination can be expressed as follows [77]:

$$I_{ph,b} = \frac{qF(1-R)\alpha L_n}{\alpha^2 L_n^2 - 1} \left(\alpha L_n - \frac{\frac{SL_n}{D_n} \left[\cosh\left(\frac{d^*}{L_n}\right) - \exp(-\alpha d^*) \right] + \sinh\left(\frac{d^*}{L_n}\right) + \alpha L_n \exp(-\alpha d^*)}{\frac{SL_n}{D_n} \sinh\left(\frac{d^*}{L_n}\right) + \cosh\left(\frac{d^*}{L_n}\right)} \right), \quad (4)$$

where F is the photon flux, R is the reflection coefficient, S is the surface recombination velocity, L_n is the minority carrier (electron) diffusion length, D_n is the electron diffusion coefficient, d^* is the thickness of the quasi-neutral region base, since the space charge region (SCR) width for the modeled structures did not exceed $1 \mu\text{m}$, it follows that $d^* \simeq d_p$.

The recombination rate affects the value of L_n and, according to the SRH model, depends on trap concentrations, capture cross-sections of electrons and holes, temperature, the Fermi level E_F location, and defect levels. Temperature also affects the values of α and D_n . In turn, the position of E_F within the band gap depends on temperature and doping level. Fig. 4 shows the calculated by using SCAPS temperature and concentration dependence of the Fermi level in the base of the investigated structure. In addition, this figure shows the positions of the levels associated with

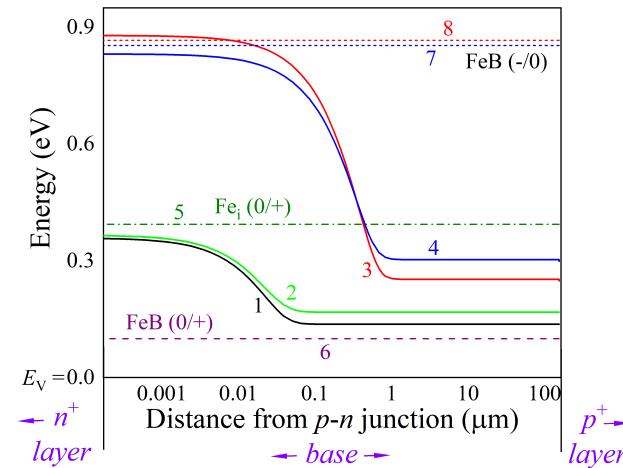


Figure 4: The location of the Fermi level (curves 1–4) in the base of the n^+ - p - p^+ structure as a function of distance from p - n junction. The zero energy value corresponds to the top of the valence band. Also shown are the locations of the donor ($0/+$) levels for the interstitial iron atom Fe_i (5) and the FeB pair (6) and the acceptor ($-/0$) level for the FeB pair (7, 8). $T, K: 290 (1, 3, 8), 340 (2, 4, 7)$. $N_B, \text{cm}^{-3}: 10^{17} (1, 2), 10^{15} (3, 4, 7, 8)$.

interstitial iron and the FeB pair. It is worth noting that Fe_i acts as a deep center; the donor state of the Fe_iB_s pair shows only negligible recombination activity, while the presence of the acceptor state Fe_iB_s causes the carrier lifetime to be doping-dependent under low injection conditions [39].

The relationship between N_B and E_F is the key factor in the influence of doping level on the sensitivity of PVPs to iron presence. Specifically, the rate of SRH recombination — and consequently, variations in PVPs 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 [60, 61]. 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 PVPs 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 [58], the concentration of ionized impurities influences charge carrier mobility and, consequently, the diffusion coefficient D_n , diffusion length L_n , and photovoltaic 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 PVPs 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.

In our opinion, the change in sign and the monotonic decrease of ϵI_{SC} with increase in doping level value reflect the change in recombination activity caused by the Fermi level shift. It should be noted that at low boron concentrations, E_F in all points of the base is located below the donor level of Fe_i , while at $N_B > 10^{16} \text{ cm}^{-3}$, they intersect in the vicinity of the p - n junction — see Fig. 4. The weak dependence on base thickness indicates that the second term in parentheses in Eq. (4) is significantly smaller than the first. In addition, when comparing monochromatic and solar illumination, the latter generates a significantly larger number of non-equilibrium carriers in the emitter due to shorter-wavelength photons. As a result, the emitter current under AM1.5 illumination increases, which, as shown in Eq. (3), leads to a decrease in ϵI_{SC} value.

Fig. 5 illustrates the alterations in the short-circuit current, both observed in experimental studies and calculated for structures with identical base parameters. It should be noted that the figure shows simulation results obtained at various levels of illumination, confirming that ϵI_{SC} is independent of W_{ill} .

One can see that the theoretical dependencies of ϵI_{SC} on iron concentration and temperature qualitatively agree with the experimental results. To achieve quantitative agreement, a correction factor of $C_{\text{cor}} = 1.4$ must be applied:

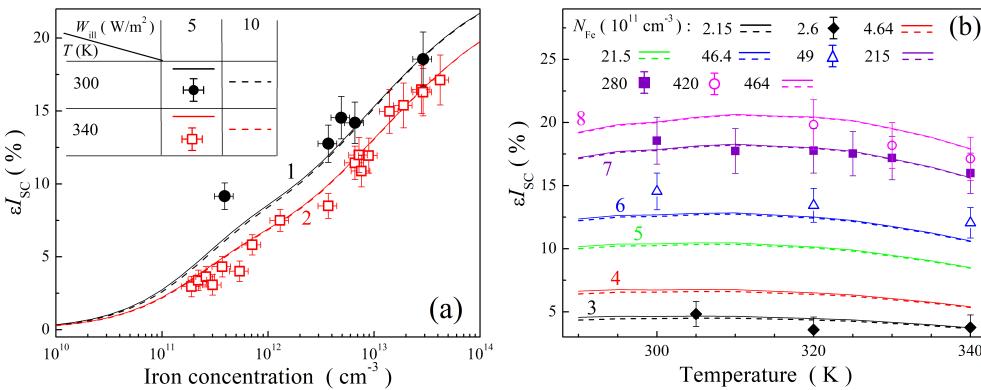


Figure 5: Relative changes in short-circuit current caused by a complete dissociation of Fe_iB_s pairs as a function of iron concentration (a) and temperature (b) for SSC with $d_p = 380 \mu m$ and $N_B = 1.36 \times 10^{15} cm^{-3}$ in the case of monochromatic (940 nm) illumination. The marks are the experimental results (divided by factor $C_{cor} = 1.4$), the lines are the simulation results. W_{ill} , W/m^2 : 5 (marks and solid lines), 10 (dotted lines). T , K (panel a): 300 (1, circles), 340 (2, squares). N_{Fe} , $10^{11} cm^{-3}$ (panel b): 2.15 (curves 3), 2.6 (diamond marks), 4.64 (4), 21.5 (5), 46.4 (6), 49 (triangles), 215 (7), 280 (squares), 420 (circles), 464 (8).

the experimentally obtained value $\varepsilon I_{SC,\text{exp}}$ should be replaced by $\varepsilon I_{SC,\text{exp}}/C_{\text{cor}}$ — as illustrated in Fig. 5. This methodology is frequently cited in the literature [26] and is associated with correcting specific systematic errors in simulations.

As mentioned above, one of the primary objectives of this study is to assess the feasibility of utilizing changes in PVPs resulting from the dissociation of FeB pairs to estimate iron concentration. One of the most promising approaches in this regard is the application of machine learning algorithms. In this context, εI_{SC} is expected to serve as one of the features. It is worth noting that a popular preprocessing technique involves standardizing feature values, where the distribution of each feature is transformed to have a mean of zero and a standard deviation of one. This approach ensures that multiplying the entire array of εI_{SC} values by a constant does not affect the resulting normalized values.

In our case, simulation errors may arise because certain factors present in actual SSCs were not accounted for in the calculations, specifically:

- the possible influence of series and shunt resistances;
- the antireflective SiO_2 and passivating Si_3N_4 layers on the front surface induce a spectral dependence in reflectance, corresponding calculations necessitating the consideration of multiple reflections [78];
- the shading caused by electrodes;
- the presence of defects unrelated to iron.

Overall, the results indicate that relative changes in short-circuit current following the complete dissociation of FeB pairs can be used to estimate iron concentration: εI_{SC} depends monotonically on N_{Fe} , and its values can be pretty significant. In this context, determining the amount of impurity atoms is more appropriately conducted using PVPs obtained under monochromatic illumination, as this method offers greater sensitivity (response amplitude of εI_{SC}). However, it should be noted that for low iron concentrations ($N_{Fe} < 10^{11} cm^{-3}$) and solar cells with boron concentrations in the base around $10^{16} cm^{-3}$, this approach appears to be unproductive. At these levels, there are blind spots in determining impurity metal concentrations.

3.2. Open-circuit voltage

Figure 7 presents the characteristic simulation results of open-circuit voltage changes due to the dissociation of FeB pairs. Figures S7–S12 in the Supplementary Material show additional εV_{OC} dependencies. Notably, the changes in V_{OC} value are almost an order of magnitude smaller than the values observed for I_{SC} . Moreover, differences in the behavior of open-circuit voltage changes as a function of iron concentration at low ($N_B < 2 \times 10^{16} cm^{-3}$) base doping levels in the cases of monochromatic and AM1.5 illumination are noteworthy. Under solar illumination, εV_{OC} values are negative, and the εV_{OC} (N_{Fe}) dependency is non-monotonic — see figs. 6a, 6b. Additionally, the base thickness significantly impacts the iron concentration, which correlates with the minimum εV_{OC} value (Fig. 6a). When illuminated by photons with a wavelength of 940 nm, εV_{OC} values are positive and increase monotonically with iron

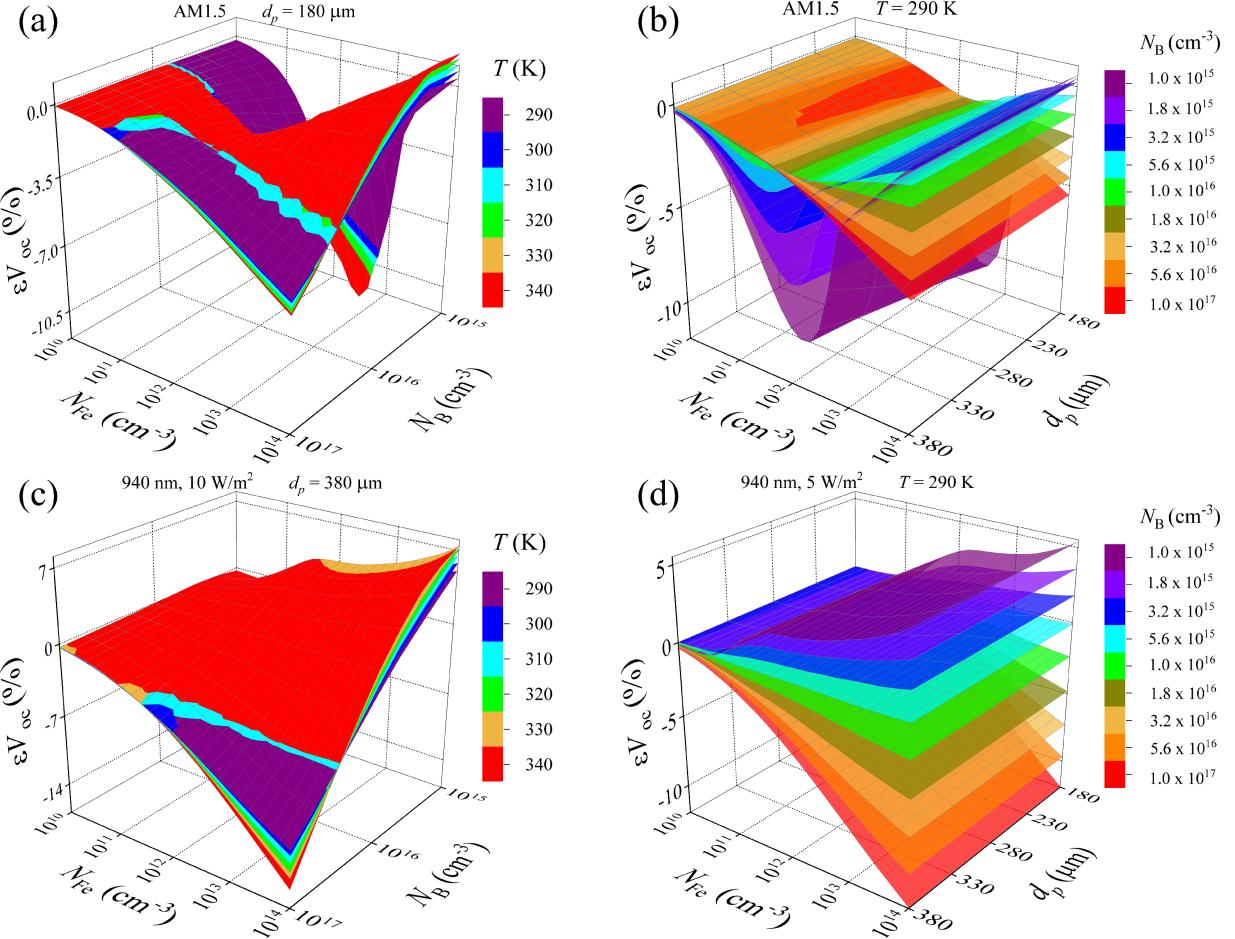


Figure 6: Relative changes in open-circuit voltage caused by a complete dissociation of Fe_iB_s pairs as a function of iron concentration and doping level (panels a and c) or base depth (b, d). Illumination: AM1.5 (a, b), 940 nm 10 W/m^2 (c), 940 nm 5 W/m^2 (d). T, K : 290 (b, d). Different surfaces correspond to different temperatures (a, c) and doping levels (b, d).

concentration. As boron concentration increases, the behavior of ϵV_{OC} (N_{Fe}) becomes similar, regardless of the type of illumination: the relative changes in open-circuit voltage during the rebuilding of iron-containing defects are negative and increase monotonically in absolute value with increasing both N_{Fe} and N_{B} . Furthermore, changes in V_{OC} are more significant under monochromatic illumination, similar to the case of the short-circuit current.

The effect of temperature on ϵV_{OC} also depends on the base doping level: as N_{B} increases, the temperature coefficient of ϵV_{OC} gradually shifts from positive to negative. This trend is observed for both AM1.5 and 940nm illumination, as shown in Figs. S9, 6a, and 6b. The impact of d_p on changes in open-circuit voltage is more significant than the effect observed for ϵI_{SC} . However, base thickness is not a determining factor for ϵV_{OC} ; it mainly affects low doping levels and temperatures, as shown in Figs. S9, S11, and S12. Another difference between the behavior of ϵV_{OC} and ϵI_{SC} is the former dependence on monochromatic illumination intensity. At $W_{\text{ill}} = 10 \text{ W}/\text{m}^2$, changes in open-circuit voltage are less significant, with differences increasing as iron concentration decreases and showing weak temperature dependence.

Understanding the features of ϵV_{OC} requires recalling that the open-circuit voltage depends not only on the photocurrent but also on the saturation current I_0 and the ideality factor, which in turn are determined by the state of the defect subsystem and other parameters that varied in simulation [37, 75]. In the case of simplified single-diode

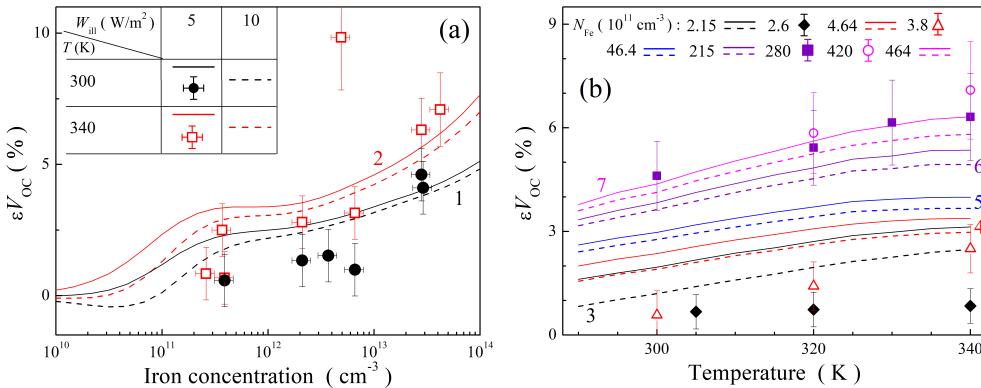


Figure 7: Relative changes in open-circuit voltage caused by a complete dissociation of Fe_iB_s pairs as a function of iron concentration (a) and temperature (b) for SSC with $d_p = 380 \mu\text{m}$ and $N_B = 1.36 \times 10^{15} \text{ cm}^{-3}$ in the case of monochromatic (940 nm) illumination. The marks are the experimental results, the lines are the simulation results. W_{ill} , W/m^2 : 5 (marks and solid lines), 10 (dotted lines). T , K (panel a): 300 (1, circles), 340 (2, squares). N_{Fe} , 10^{11} cm^{-3} (panel b): 2.15 (curves 3), 2.6 (diamond marks), 4.64 (4), 3.8 (triangles), 46.4 (5), 215 (6), 280 (squares), 420 (circles), 464 (7).

model [75]:

$$V_{OC} = nkT \left[\ln \left(\frac{I_{\text{ph}}}{I_0} \right) + 1 \right]. \quad (5)$$

Similar to the photocurrent, we can express I_0 as the sum of the currents from the base and the emitter [76]:

$$I_0 = I_{0,e} + I_{0,b}, \quad (6)$$

and the second term can be expressed as follows [77]:

$$I_{0,b} = \frac{qn_i D_n}{N_B L_n} \cdot \frac{\frac{D_n}{SL_n} \sinh \left(\frac{d_p}{L_n} \right) + \cosh \left(\frac{d_p}{L_n} \right)}{\sinh \left(\frac{d_p}{L_n} \right) + \frac{D_n}{SL_n} \cosh \left(\frac{d_p}{L_n} \right)}, \quad (7)$$

where n_i is the intrinsic carrier concentration. The last equation explains the observed dependence of εV_{OC} on the base thickness.

It was shown [38, 37] previously that changes in the ideality factor during restructuring $\text{Fe}_i\text{B}_{\text{Si}} \rightleftharpoons \text{Fe}_i + \text{B}_{\text{Si}}$ do not exceed a few percent. This n slight variation, combined with the logarithmic dependence of V_{OC} on I_{ph} as shown in Eq. (5), explains the small absolute values of εV_{OC} .

Schmidt [39] attributes the non-monotonic dependence of εV_{OC} (N_{Fe}) (Fig. 6b) to the significantly higher injection level in the cell base under open-circuit conditions compared to short-circuit conditions. Overall, the results support this hypothesis. In fact, for monochromatic illumination with significantly lower intensity, the injection level remains below the crossover point [39] throughout the $I-V$ curve, which results in the absence of a minimum in the εV_{OC} (N_{Fe}) dependence.

The data presented in Fig. 7 compare the experimental and simulation results. Overall, the results in both cases are qualitatively consistent. However, to ensure that the absolute values are consistent, a correction factor dependent on iron concentration must be used. According to the data, C_{cor} is less than 1 for low values of N_{Fe} and greater than 1 for high values. By the way, Schubert et al. [26] also observed such dependence of the correction factor.

It is believed [75] that the main effect of metals on the V_{OC} values can be determined by shunt formation. However, SCAPS does not account for the effect of shunt resistance, which we believe is the primary reason for the discrepancies between experimental and simulated values.

In summary, using relative changes in open-circuit voltage due to FeB pair dissociation is less convenient for estimating iron concentration compared to εI_{SC} . It is because of the smaller absolute values of εV_{OC} , the non-monotonic dependence of εV_{OC} on N_{Fe} under certain conditions, and the need for precise control over the intensity

of monochromatic illumination. However, using ϵV_{OC} as an additional parameter alongside ϵI_{SC} can significantly enhance the accuracy of iron concentration measurements for $N_{Fe} < 10^{11} \text{ cm}^{-3}$ and $N_B = (1 - 5) \times 10^{15} \text{ cm}^{-3}$ under AM1.5 illumination. In this case, the dependence of ϵV_{OC} on N_{Fe} is sufficiently sharp (Fig. 6b), and ambiguity in associating specific ϵV_{OC} values with iron concentration can be resolved by the monotonic behavior of ϵV_{OC} in this range. Notably, these boron concentrations are most relevant to typical real SSCs.

3.3. Fill factor

The fill factor is another defining term in the overall behavior of a solar cell. FF is the ratio of the maximum obtainable power to the product of short circuit current and open-circuit voltage. In general, FF depends on both I_{SC} and V_{OC} . However, it can be shown that it is mainly determined by the V_{OC} value. Indeed, it is shown [75] within the single-diode model

$$FF \approx \frac{v_{OC} - \ln(1 + v_{OC})}{v_{OC} + 1}, \quad (8)$$

with v_{OC} being the normalized open-circuit voltage $v_{OC} = qV_{OC}/nkT$. Another well-known empirical relation for the maximum achievable fill factor of a solar cell is proposed by Green [79, 80]:

$$FF \approx \frac{v_{OC} - \ln(0.72 + v_{OC})}{v_{OC} + 1}. \quad (9)$$

Thus, any factors that affect V_{OC} also impact the FF . However, since V_{OC} appears in both the numerator and denominator of Eqs. (8)-(9), the resulting changes in the fill factor are expected to be smaller than those in the open-circuit voltage.

Recently, Bothe et al. [81] proposed explicit expressions for the FF in terms of other key solar cell parameters. Specifically, for p -type SSCs and intrinsic limits, the parameterization can be expressed as follows:

$$FF = \frac{90.4924}{d_p^{0.00220}} \left[0.9478 + \frac{0.0519}{1 + \left(\frac{\log N_B}{17.3739 d_p^{-0.0093}} \right)^{76.3}} \right], \quad (10)$$

where d_p is expected to be in micrometers. Additional recombination (e.g., Shockley–Read–Hall) leads to a decrease in FF value [81].

Figs. S13–S16 in the Supplementary Material, along with Fig. 8, illustrate how the fill factor varies with iron defect variability. The following features of ϵFF can be identified from the presented data:

- The changes in the fill factor are the smallest among the parameters considered, with maximum ϵFF values not exceeding 10%;
- At low boron concentrations ($N_B < 10^{16} \text{ cm}^{-3}$), 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 BaZrSe₃–based perovskite solar cells [6];
- At low boron concentrations, the change in fill factor value is positive and, in contrast to ϵV_{OC} and ϵI_{SC} , AM1.5 illumination causes more significant changes in ϵFF than monochromatic illumination. At high boron concentrations, the ϵFF is negative and does not exceed 4%;
- The absolute value of ϵFF increases, regardless of the value sign, with temperature increases;
- Increasing the base thickness leads to a decrease in ϵFF (a reduction in the fill factor with increasing d_p is expected according to (10)). Additionally, this results in a shift of the ϵFF (N_{Fe}) dependence towards lower iron concentrations. The impact of d_p is more pronounced at low boron concentrations and in the case of AM1.5 illumination;
- In the case of monochromatic illumination, the light intensity significantly affects the relative changes in the fill factor (ϵFF can vary by a factor of 2 when W_{ill} changes from 5 to 10 W/m²). This impact is influenced by both iron concentration (which can even change the sign of the effect) and temperature.

Fig. 9 shows that the experimental dependencies of ϵFF (N_{Fe}) and ϵFF (T) align well with the calculated values.

Figure 9 shows that the experimental dependencies ϵFF (N_{Fe}) and ϵFF (T) are in good agreement with the calculated values. In our opinion, the quantitative agreement is limited by the relatively low accuracy of ϵFF

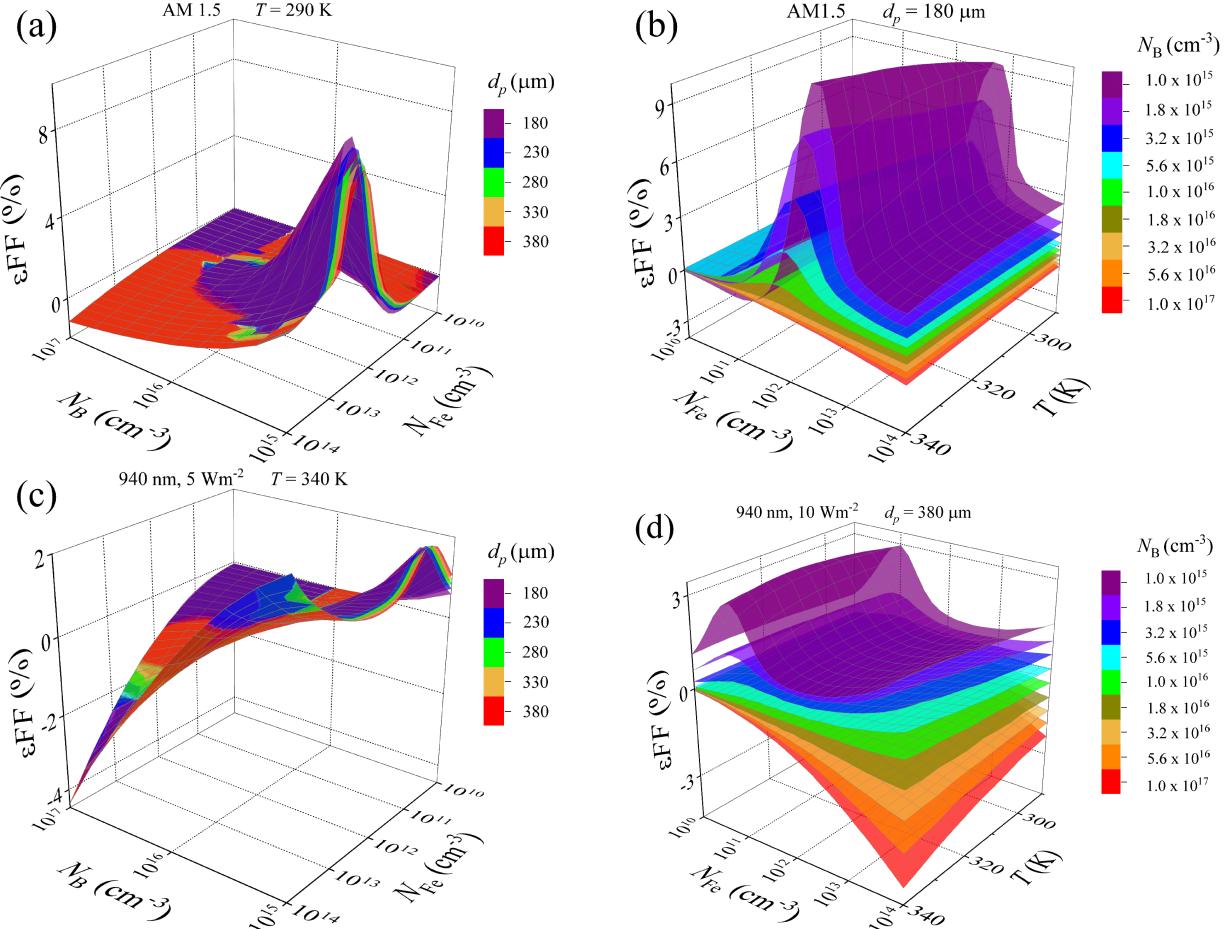


Figure 8: Relative changes in fill factor caused by a complete dissociation of Fe_xB_y pairs as a function of iron concentration and doping level (panels a and c) or temperature (b, d). Illumination: AM1.5 (a, b), 940 nm 5 W/m^2 (c), 940 nm 10 W/m^2 (d). T, K : 290 (a), 340 (c). $d_p, \mu\text{m}$: 180 (b), 380 (d). Different surfaces correspond to different base depths (a, c) and doping levels (b, d).

measurements and the dependence of fill factor on series and shunt resistances [79, 80], which were not considered in the simulation.

The observed characteristics of ϵFF suggest that the fill factor is considerably less suitable for estimating iron concentration in SSCs than the short-circuit current and open-circuit voltage. ϵFF can serve as an auxiliary parameter to refine N_{Fe} ; however, if monochromatic illumination is used, light intensity must be controlled with high precision.

51 3.4. Solar cell efficiency

52 Solar cell efficiency depends on all the photovoltaic conversion parameters previously discussed:

$$54 \quad \eta = \frac{I_{\text{SC}} V_{\text{OC}} \text{FF}}{W_{\text{ill}} A}, \quad (11)$$

55 where A is the illuminated area of the solar cell. Considering the differential of Eq. (11), a cumulative effect on the
56 relative changes in efficiency can be anticipated.

57 Considering the differential of formula (11):

$$58 \quad d\eta = \frac{dI_{\text{SC}}}{I_{\text{SC}}} + \frac{dV_{\text{OC}}}{V_{\text{OC}}} + \frac{d\text{FF}}{\text{FF}}, \quad (12)$$

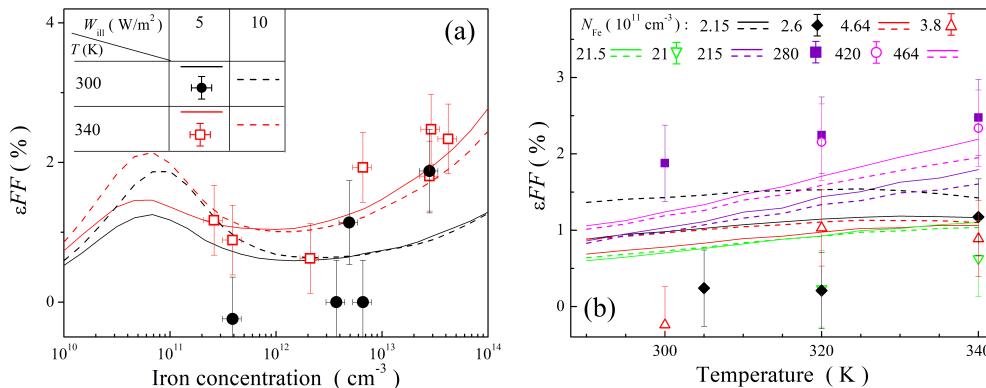


Figure 9: Relative changes in fill factor caused by a complete dissociation of Fe_xB_y pairs as a function of iron concentration (a) and temperature (b) for SSC with $d_p = 380 \mu\text{m}$ and $N_B = 1.36 \times 10^{15} \text{ cm}^{-3}$ in the case of monochromatic (940 nm) illumination. The marks are the experimental results, the lines are the simulation results. W_{ill} , W/m^2 : 5 (marks and solid lines), 10 (dotted lines). Different lines and marks correspond to different temperatures (a) or N_{Fe} values (b) — see legends.

a cumulative effect on the relative changes in efficiency can be anticipated. Fig. 10 illustrates the simulation results for the solar cell efficiency, while Figs. S17–S20 offer additional details in the Supplementary Material.

The data indicate that the primary features of the ϵ_{η} dependencies on solar cell parameters and temperature align with those observed for ϵI_{SC} . However, a few differences are evident: 1) the amplitude of ϵ_{η} is enhanced, reaching up to 50% for AM1.5 and 200% for 940 nm; these results align with the expectations from Eq. (12) and make SC efficiency more convenient for iron concentration estimating; 2) for AM1.5, in the region $N_B < 5 \times 10^{15} \text{ cm}^{-3}$, a non-monotonic dependence of $\epsilon_{\eta}(N_{Fe})$ is observed, rendering it impossible to use relative changes in efficiency as the sole parameter for iron concentration estimating under specified conditions; 3) the existing dependence of ϵ_{η} on the intensity of the monochromatic illumination is weak, which does not prevent the use of ϵ_{η} for determining N_{Fe} , even with not very precise W_{ill} measurements; 4) the temperature dependence of ϵ_{η} is weaker than that of ϵI_{SC} .

Fig. 11 shows the experimental and simulated values of changes in the efficiency of the solar cell with a $380 \mu\text{m}$ base thickness and a doping concentration of $1.36 \times 10^{15} \text{ cm}^{-3}$. When presenting the experimental data, the same correction factor, $C_{\text{cor}} = 1.4$, was applied as in the case of the short-circuit current. The data align closely, indicating that the inaccuracies typical for V_{OC} and FF do not significantly contribute.

The revealed characteristics of ϵ_{η} indicate that this PVP is entirely suitable for estimating iron concentration.

Two key metrics were used to identify the solar cell parameter whose changes, resulting from the $\text{Fe}_x\text{B}_{Si} \rightleftharpoons \text{Fe}_x + \text{B}_{Si}$ 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 ϵ_{FF} , ϵV_{OC} , and ϵ_{η} (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 ϵ_{η} 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 ϵ_{η} 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.

3.5. Photovoltaic parameters correlation

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

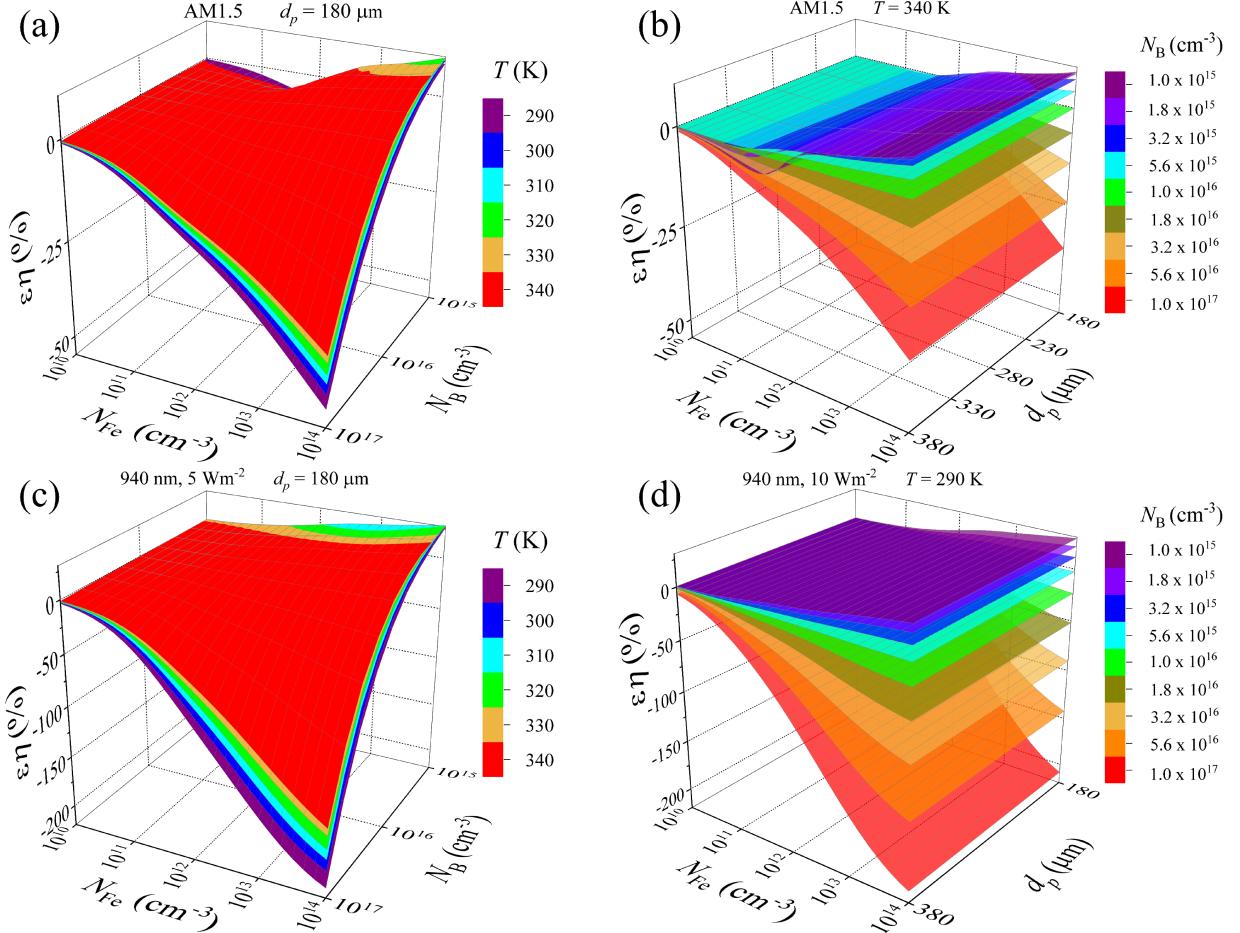


Figure 10: Relative changes in SSC efficiency caused by a complete dissociation of Fe_iB_s pairs as a function of iron concentration and doping level (panels a and c) or base depth (b, d). Illumination: AM1.5 (a, b), 940 nm 5 W/m^2 (c), 940 nm 10 W/m^2 (d). T, K : 290 (d), 340 (b). $d_p, \mu\text{m}$: 180 (a, c). Different surfaces correspond to different temperatures (a, c) and doping levels (b, d).

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 $(T, d_p, N_B, \varepsilon I_{\text{SC}})$. Evidently, incorporating additional information, such as changes in efficiency ($\varepsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_B, \varepsilon I_{\text{SC}}, \varepsilon\eta)$, 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 $(T, d_p, N_B, \varepsilon I_{\text{SC}}, \varepsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_B, \varepsilon I_{\text{SC}})$.

Analyzing their correlations can help evaluate the independence of the parameters. Fig. 12 presents the Pearson correlation coefficients calculated for all parameter sets. Additionally, it shows the correlation between iron concentration and each input parameter. It's worth noting that the N_{Fe} and N_B values in the logarithmic scale were used in calculations. It is a common approach for quantities that span several orders of magnitude [82].

Firstly, it is noteworthy that, as indicated by the obtained data, the value of N_{Fe} exhibits a weak correlation with each descriptor. Consequently, using any parameter in isolation from others is not feasible for precise iron concentration estimation. Regarding the descriptors associated with photovoltaic energy conversion, all of these

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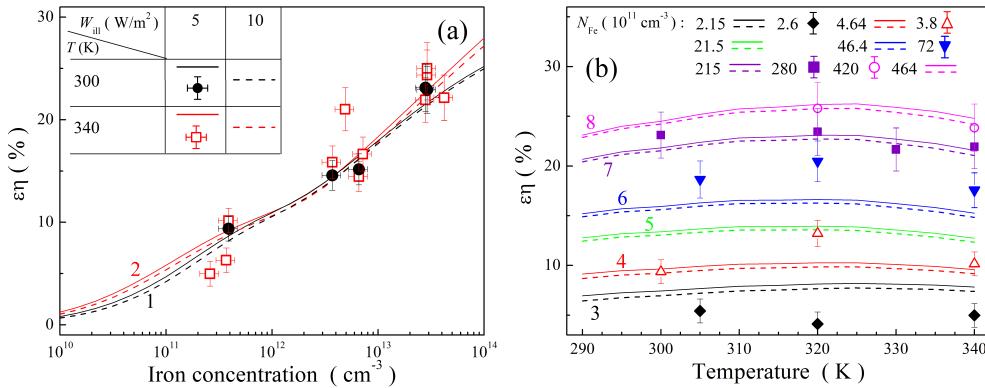


Figure 11: Relative changes in SSC efficiency caused by a complete dissociation of Fe_iB_s pairs as a function of iron concentration (a) and temperature (b) for SSC with $d_p = 380 \mu\text{m}$ and $N_B = 1.36 \times 10^{15} \text{ cm}^{-3}$ in the case of monochromatic (940 nm) illumination. The marks are the experimental results (divided by factor $C_{cor} = 1.4$), the lines are the simulation results. W_{ill} , W/m^2 : 5 (marks and solid lines), 10 (dotted lines). T , K (panel a): 300 (1, circles), 340 (2, squares). N_{Fe} , 10^{11} cm^{-3} (panel b): 2.15 (curves 3), 2.6 (diamond marks), 3.8 (open triangles), 4.64 (4), 21.5 (5), 46.4 (6), 72 (filled triangles), 215 (7), 280 (squares), 420 (circles), 464 (8).

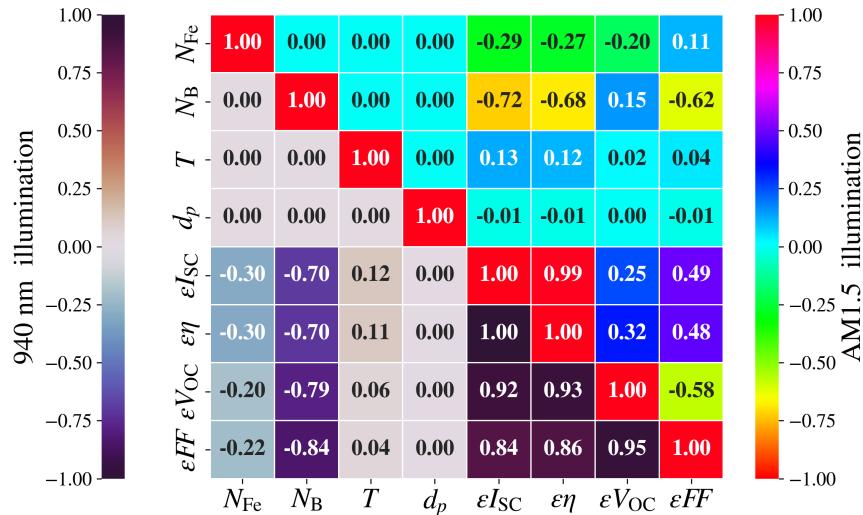


Figure 12: Correlation plot of photovoltaic conversion parameters and solar cell characteristics. Data above and below the main diagonal correspond to AM1.5 and 940 nm (5 W/m^2) illumination, respectively.

parameters correlate strongly with the base doping level, except for open-circuit voltage under AM1.5 illumination. In addition, these parameters are substantially correlated with each other, which is particularly noticeable when using monochromatic illumination. Thus, augmenting the descriptor set by incorporating relative changes in additional photovoltaic parameters introduces substantial redundancy in the input data.

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 [83]. 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 PVPs 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

Table 2

PSA results for sets of variables that serve to estimate the iron concentration in SSC. The numbers represent the ratio of information variance associated with each principal component when using AM1.5 illumination / 940 nm illumination.

set of descriptors	Explained Variance Ratio (%)						
	PC0	PC1	PC2	PC3	PC4	PC5	PC6
($T, d_p, N_B, \epsilon I_{SC}$)	43.23/42.80	25.00/25.00	25.00/25.00	6.70/7.20	—	—	—
($T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta$)	52.39/52.46	20.00/20.00	20.00/20.00	7.48/7.51	0.13/0.03	—	—
($T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}$)	44.40/59.02	18.78/16.73	16.67/16.67	16.46/6.28	3.61/1.29	0.08/0.01	—
($T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}, \epsilon FF$)	43.29/63.24	22.59/14.41	14.29/14.29	14.19/5.65	4.29/1.95	1.35/0.46	0.002/0.01

the solar cell's base parameters and temperature, no excessive information is present (in the case of the descriptor set ($T, d_p, N_B, \epsilon I_{SC}$), 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 ($T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}, \epsilon FF$) 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 PVPs, it is advisable to apply PCA to transform the original data. Thus, the simultaneous use of $\epsilon\eta$ 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%).

4. Conclusion

We have provided the results of modeling the impact of variations in the state of iron impurities on the photovoltaic parameters of silicon solar cells with different base properties under various external conditions (temperature, intensity, and spectral composition of illumination). The simulation results have been compared with experimental data.

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. It is shown that short-circuit current is the most suitable parameter for iron quantification, as variations in I_{SC} value during the $Fe_iB_{Si} \rightleftharpoons Fe_i + B_{Si}$ transformation can be effectively utilized. Determining PVPs 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.

It has been shown that the potential accuracy of estimating iron concentration depends on the doping level of the base: at a boron concentration around $10^{16} cm^{-3}$, it is minimal, while decreasing or increasing this value enhances the response of I_{SC} to the presence of iron. Furthermore, the accuracy of N_{Fe} determination is significantly influenced by the availability of precise information on the doping level of the base, as well as the accuracy of estimating the intensity of monochromatic illumination, especially when using $\epsilon\eta$ and ϵV_{OC} .

At the same time, $\epsilon\eta$ and ϵV_{OC} can serve as additional parameters for refining the determination of iron concentration. In our opinion, for estimating iron concentration through changes in PVP values due to variability in iron-related defects, it is advisable to use a set of ($T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta$) or ($T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}$). Furthermore, it has been demonstrated that iron-induced changes in various PVPs are correlated. Therefore, if iron concentration estimation is performed using changes in multiple PVPs, applying Principal Component Analysis is advisable. This data transformation reduces the number of variables while preserving the maximum variance information and accelerating calculations.

Our study lays the groundwork for developing an efficient, express, cost-effective method for monitoring iron impurity concentrations in silicon solar cells. This approach relies on current-voltage measurements and can be easily

incorporated into the standard characterization procedure for silicon photovoltaic devices. Through simulations and experiments, we have identified a key metric for quantifying iron impurities (short-circuit current) and determined which factors significantly (base doping level, temperature) and insignificantly (base thickness) influence the response of solar cells to iron-related defect rearrangements. These findings should be considered when implementing the method in practice. Our approach allows for the simultaneous determination of the concentration of iron impurities along with the standard solar cell parameters (such as short-circuit current, open-circuit voltage, and nominal power), all without needing additional equipment. The suggested and verified approach advances our understanding of impurity effects and paves the way for improved solar cell reliability.

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Supplementary data

Supplementary data to this article can be found online at <http://surl.li/qneich>

Data availability

Data will be made available on request.

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Oleg Olikh reports financial support was provided by National Research Foundation of Ukraine. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.