# **A Deep Neural Network Approach to Estimate Iron Contamination of a Solar Cell Using Photovoltaic Parameters**

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# **SUMMARY OF THE ABSTRACT**

Using an approach based on deep neural networks (DNN), the contamination of a solar cell with iron was estimated using the ideality factor. In this research, the assessment was additionally performed on photovoltaic parameters.

The I-V characteristics under illumination were modeled. After approximating the I-V characteristics, the photovoltaic parameters were determined. After creating the database, we set up and trained deep neural networks. Tested networks using synthetic and experimental I-V characteristics. The calculations were performed for the structure at different values of temperature, base thickness, boron and iron dopant concentrations. We considered 2 neural networks with different input layers, which were created in the Keras API framework. To optimize the networks, we determined the optimal values of 12 hyperparameters. To assess the quality of trained networks, we used MSRE, Pearson's correlation coefficient , and determination coefficient .

More than 95 000 I-V characteristics of silicon structures with different base thicknesses , boron doping levels , temperatures , and iron concentrations were modeled. The cases of the structure under sunlight and monochromatic light illumination are considered, it is taken into account that impurity iron atoms can be in the interstitial state and as part of the FeB pair. MSRE predictions of iron concentration can reach . The highest accuracy of the estimates is observed for structures with a doping level that corresponds to the values used during training. The best predictive results are achieved when applied to networks with relative changes in all parameters of photovoltaic conversion. Possible ways to improve the estimation accuracy by modifying the dataset and applying retraining of standard image processing networks are considered.

# **APPLICABLE TOPIC AND SUB-TOPIC NUMBER**

TOPIC 1: Silicon Materials and Cells

1.4 Characterisation & Modelling of Si Cells

# **EXPLANATORY PAGES**

# **AIM AND APPROACH**

The aim was to develop and configure (determine the optimal values of hyperparameters) deep neural networks designed to predict the concentration of impurity iron in silicon structures by the values of the doping level, base thickness, temperature, and photovoltaic conversion characteristics. Among all possible hyperparameters, we chose the following: number of hidden layers, number of nodes in the first hidden layer, batch size, type of activation function for hidden layers, type of optimizer, learning rate, number of epochs, data preprocessing method, type of regularization function, regularization rate, thinning rate, type of initialization of weights. We considered 5 configurations of hidden layers: 1) all hidden layers consist of the same number of nodes; 2) six hidden layers, in each subsequent layer the number of nodes decreases by 10% of the number of nodes in the first layer; 3) ten layers, in which the number of neurons uniformly decreases from 100% (first layer) to 10% (last layer); 4) two mirrored trapezium configurations; 5) Two consecutive configurations of #2. To quantify the prognostic properties of DNNs on the training set, we used a 5-fold cross-validation. We considered the relative changes of the photovoltaic parameters: short-circuit current , open-circuit voltage , fill factor and efficiency . I-V characteristics were calculated using the one-dimensional modeling software package SCAPS. During the modeling, we calculated the position of the Fermi level, which was used to assess the spatial distribution of defects. The simulation was performed in the voltage range from zero voltage to no-load voltage. The solar cell was illuminated either with sunlight (AM1.5 spectrum, 1000 illumination power, which corresponds to standard conditions), or with monochromatic light (940 nm, 4 , which coincides with the case when the light-emitting diode SN-HPIR940nm-1W is used for illumination). In addition, it was necessary to demonstrate the ability of the developed neural networks to determine the concentration of iron based on both synthetic and experimentally measured I-V characteristics.

# **SCIENTIFIC INNOVATION AND RELEVANCE**

The recombination processes associated with defects (intrinsic and impurity) are extremely important for understanding the properties of solar cells, as they often limit the efficiency of photovoltaic devices. However, the physical parameters that control these processes can be extremely difficult to measure, requiring special methods and sample preparation. Non-destructive methods aimed at estimating the concentration of impurities in semiconductor structures are important from the applied point of view. The problem of the multivariate relationship between recombination center concentration and I-V parameters, which is one of the main obstacles to the development of a user-friendly and rapid method, can be easily solved by DNNs.

# **RESULTS (OR PRELIMINARY RESULTS) AND CONCLUSIONS**

The largest error is observed in the case when the test set was distorted using doping values that were not found in the training set. For the monochromatic light, using the full data set (training + test) for training shows almost no improvement over the data set without the test component. For the solar spectrum, on the other hand, training on the full dataset has significantly increased efficiency. The combination of photovoltaic parameters may be the topic of further research. This hypothesis comes from a previous research on the ideality factor, where the use of several ideality factors (after FeB pair decay and at equilibrium) was more effective than using only one ideality factor to predict.

We also investigated the applicability of the developed DNNs to real solar cells (BSF and PERC). The applicability of the created DNNs is determined by the fulfillment of the Shockley-Reed-Hall (SCR) condition. In addition, the base must be doped with boron. If the base is not doped with boron, the simulation model should be changed. If other defects are present in the solar cell and also cause intensive recombination of the SCR, the calculation model should be more complex. The next step in the research may be the characterization of defects in photovoltaic cells. In our opinion, there are two main ways to improve the method. The first is related to the use of a better data set for training DNNs. This set can be generated either by using 3D barrier structure simulators (e.g., SILVACO TCAD or SENTAURUS TCAD) or by experimental measurements of I-V characteristics on a wide range of real solar cells. The second way is related to improving the functioning of DNNs, and in this case, the most promising approach seems to be the use of a pre-training approach. For example, a small set of structure parameters and measurement results can be multiplied and transformed into an image. After that, ready-made (trained, optimized) DNNs (for example, VGG16) can be used for image recognition.

Далі буде використана тема ця:

1) «Deep Learning for Impurity Detection in Silicon Photovoltaic Cells: Optimization and Characterization of Doping Level, Base Thickness, Temperature, and Photovoltaic Properties»

Але ще можливі такі теми:

2) «Optimizing Deep Neural Networks for Impurity Detection in Silicon Photovoltaic Cells: An Exploration of Hyperparameters and Recombination Processes»

3) «Predicting Impurity Concentration in Silicon Photovoltaic Cells using Deep Learning: Optimization of Hyperparameters and Analysis of Recombination Processes»

4) «Optimizing Photovoltaic Performance through Hyperparameter Tuning of Deep Neural Networks for Impurity Detection in Silicon Solar Cells»

# **Deep Learning for Impurity Detection in Silicon Photovoltaic Cells: Optimization and Characterization of Doping Level, Base Thickness, Temperature, and Photovoltaic Properties**

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# **SUMMARY OF THE ABSTRACT**

In this research, the contamination of a solar cell with iron was estimated by utilizing deep neural networks (DNNs) and evaluating the ideality factor. Additionally, the assessment was conducted on various photovoltaic parameters

In this study, the I-V characteristics of a structure under illumination were modeled and used to determine photovoltaic parameters. A database was created and DNNs were trained and tested using synthetic and experimental I-V characteristics. The calculations were performed at varying temperatures, base thickness, boron and iron dopant concentrations. Two neural networks with distinct input layers were developed using the Keras API framework, and optimal values for 12 hyperparameters were determined to optimize the networks. The performance of the trained networks was evaluated using metrics such as the mean square relative error MSRE, Pearson's correlation coefficient , and determination coefficient .

Over 95,000 I-V characteristics of silicon structures were modeled, with variations in base thickness , boron doping levels , temperatures , and iron concentrations . The effects of sunlight and monochromatic light illumination were taken into account, and the presence of iron impurities in both interstitial and FeB pair states were considered. The predictions of iron concentration using MSRE can reach a precision of . The highest accuracy of the estimates was observed when the doping level was close to the values used during training. The best results were achieved when the network was trained on relative changes in all parameters of photovoltaic conversion. The study also explored ways to improve the estimation accuracy through modifications to the dataset and retraining with standard image processing networks.

# **APPLICABLE TOPIC AND SUB-TOPIC NUMBER**

TOPIC 1: Silicon Materials and Cells

1.4 Characterisation & Modelling of Si Cells

# **EXPLANATORY PAGES**

# **AIM AND APPROACH**

The goal of this study was to develop DNNs and optimize them by finding the best values for the hyperparameters in order to predict the amount of impurity iron in silicon structures using doping level, base thickness, temperature, and photovoltaic conversion properties as inputs. From the available hyperparameters, the following were selected: number of hidden layers, number of nodes in the first hidden layer, batch size, activation function for hidden layers, optimizer, learning rate, number of epochs, method used for data preprocessing, regularization function, regularization rate, thinning rate, and initialization method for the weights. Five different configurations for hidden layers were evaluated: 1) all hidden layers having an equal number of nodes; 2) six hidden layers, with the number of nodes in each subsequent layer decreasing by 10% of the number of nodes in the first layer; 3) ten layers, with the number of neurons uniformly decreasing from 100% (first layer) to 10% (last layer); 4) two mirrored trapezium configurations; 5) Two consecutive configurations of #2. The ability of DNNs to make predictions on the training set was measured using a 5-fold cross-validation method. The relative changes of photovoltaic parameters, such as short-circuit current , open-circuit voltage , fill factor , and efficiency , were evaluated. I-V characteristics were computed using the SCAPS one-dimensional modeling software. The modeling process included the calculation of the Fermi level position, which was used to evaluate the spatial distribution of defects. The simulation was conducted in the voltage range from zero to no-load voltage. The solar cell was illuminated either with sunlight (AM1.5 spectrum, 1000 illumination power, which represents standard conditions) or with monochromatic light (940 nm, 4 , which corresponds to the use of the light-emitting diode SN-HPIR940nm-1W for illumination). Additionally, it was necessary to demonstrate that the developed DNNs could determine the iron concentration based on both synthetic and experimentally-obtained I-V characteristics.

# **SCIENTIFIC INNOVATION AND RELEVANCE**

The study of recombination processes caused by defects in solar cells is crucial for understanding the limitations of their efficiency. However, measuring the physical parameters that control these processes can be challenging and require specialized techniques. Non-destructive methods for determining impurity concentrations in semiconductor structures are useful in practical applications. The challenge of determining the relationship between the concentration of recombination centers and I-V parameters can be overcome using DNNs.

# **RESULTS (OR PRELIMINARY RESULTS) AND CONCLUSIONS**

The largest discrepancy is observed when the test set is distorted using doping values not found in the training set. When using monochromatic light, using the full data set (training + test) for training shows little to no improvement compared to using only the training data. However, when using the solar spectrum, training on the full dataset results in a significant increase in efficiency. The combination of photovoltaic parameters may be a topic for further research. This hypothesis arises from previous research on the ideality factor, where the use of multiple ideality factors (after FeB pair decay and at equilibrium) was found to be more effective than using a single ideality factor.

We also investigated the applicability of the developed DNNs to real solar cells (BSF and PERC). The applicability of the DNNs was determined by their compliance with the Shockley-Reed-Hall (SRH) condition. Additionally, the base layer must be doped with boron. If the base is not doped with boron, the simulation model must be altered. If other defects are present in the solar cell that also cause intensive recombination of the SRH, the calculation model must be more complex. The next step in the research could be the characterization of defects in photovoltaic cells. In our opinion, there are two main ways to improve the method. The first is to use a more robust dataset for training DNNs. This dataset can be generated either by using 3D barrier structure simulators (such as SILVACO TCAD or SENTAURUS TCAD) or by conducting experimental measurements of I-V characteristics on a diverse range of real solar cells. The second way is to improve the performance of DNNs, and in this case, the most promising approach seems to be the use of a pre-training method. For example, a small set of structural parameters and measurement outcomes can be converted into an image. Then, pre-trained and optimized DNNs (such as VGG16) can be used for image recognition.