# **Evaluating the Performance of DNNs for Iron Concentration Prediction in Silicon Solar Cells using Photovoltaic Parameters**

Olikh O.Ya., Zavhorodnii O.V.

Taras Shevchenko National University of Kyiv

[olikh@univ.kiev.ua](mailto:olikh@univ.kiev.ua), nevermor464@gmail.com

# **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.

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. Improvement methods are described, which include parameter filtering, advanced modeling, and new dependencies generated by the Fourier transform.

# **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 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 correlation 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. Different approaches can be taken to improve the method. One option is to use 3D modeling programs such as Silvaco TCAD or Sentaurus TCAD. Another interesting idea is to convert existing solar cell parameters into new parameters by creating a time-dependence of the photoelectric parameters and applying the Fourier transform. It is crucial to investigate the impact of photoelectric parameters on prediction accuracy. The efficiency (η) of a solar cell is typically determined by the short-circuit current (Isc), open-circuit voltage (Voc), and fill factor (FF). Using efficiency along with other photovoltaic parameters shouldn't improve the predictive capability of the neural network. However, this is not always the case. Such results led us to two thoughts: 1) The inclusion of the efficiency enhances the efficiency of the neural network, as Isc, Voc, FF do not fully capture the efficiency and considering input power is necessary for a complete description of the efficiency. 2) The second idea builds upon the first - using the Fourier transform to create functional but "phantom" dependencies.