

## Highlights

### **main title**

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- Proposed deep learning-based method to predict iron contamination in Si-SC by using IV curve.
- The simulated IV characteristics are used to create training and test datasets.
- The DNN's configurations are proposed.
- The mean squared relative error of prediction is up to 0.005.

## ARTICLE INFO

### Keywords:

Ideality factor

Silicon

$n^+-p-p^+$  structure

SCAPS

Iron-contamination

Machine learning

1.

In our previous work, we have shown that the SC ideality factor value ( $n$ ) can be used to estimate the iron concentration ( $N_{Fe}$ ). It should be noted that the ideality factor is quite often used to characterize the various semiconductor barrier structures. However, a defect's signature in an ideality factor is convoluted with those from so many other physical processes. As a result, obtained analytic expressions  $N_{Fe} = f(n)$  are not general and the numerous grading curves are required to determine  $N_{Fe}$ ; besides the IV measurements over a temperature range are necessary. On the other hand, in the last decade, the deep learning, which enables to solve problems without clear algorithmization, have been successfully used in various fields of theoretical and applied physics. Furthermore, materials informatics (combination of material property calculations/measurements and informatics algorithms) has been asserted to become the fourth (along with theory, simulations, and experiments) paradigm of science. The aim of this work is to apply the deep learning approach for predicting of the iron concentration from ideality factor (so to say "deep learning for deep levels"). Further, unlike in previous work, the back surface field (BSF)  $n^+-p-p^+$  structure was under consideration and the influence of the base thickness on ideality factor was taken into account as well.

As the approximation to the practical using, the paper considers a fairly simple system which consists of crystalline silicon (c-Si) SC and iron impurity. However, the system is important in practice. Silicon solar cells constitute 90% of current global production capacity and BSF is one of popular designs used for industrial mass production of c-Si SCs. Iron is a major as well as one of the most detrimental metallic impurities in c-Si SCs. The flowchart of the used heuristic approach is shown in Fig. ???. The following constituents can be distinguished. First, the dark IV characteristics are simulated for SCs with both known contaminant composition and various parameters. In our numerical simulation we applied SCAPS-1D, which widely used to model solar cells. Second, the obtained characteristic is fitted according to the double-diode model and the ideality factor is estimated. As a result of aforesaid steps, the labeled datasets were

## ABSTRACT

Defect-assisted recombination processes frequently limit the photovoltaic device performance. The low-cost and express methods of impurity contamination control are in demand at solar cell manufacturing. In this paper, we applied deep learning-based approach to extract the iron concentration in silicon solar cell from an ideality factor values.


Table 1

produced. Obviously, the labeled dataset from experimental IVs would be preferable, but it is practically difficult to find the thousands of samples with the required parameters. Third, the training of deep neural network (DNN) to estimate an iron contamination by using SC's base thickness, doping level, temperature, and ideality factor value. Fours, the DNN testing.

## 2.

In our previous work, we have shown that the SC ideality factor value ( $n$ ) can be used to estimate the iron concentration ( $N_{Fe}$ ). It should be noted that the ideality factor is quite often used to characterize the various semiconductor barrier structures. However, a defect's signature in an ideality factor is convoluted with those from so many other physical processes. As a result, obtained analytic expressions  $N_{Fe} = f(n)$  are not general and the numerous grading curves are required to determine  $N_{Fe}$ ; besides the IV measurements over a temperature range are necessary. On the other hand, in the last decade, the deep learning, which enables to solve problems without clear algorithmization, have been successfully used in various fields of theoretical and applied physics. Furthermore, materials informatics (combination of material property calculations/measurements and informatics algorithms) has been asserted to become the fourth (along with theory, simulations, and experiments) paradigm of science. The aim of this work is to apply the deep learning approach for predicting of the iron concentration from ideality factor (so to say "deep learning for deep levels"). Further, unlike in previous work, the back surface field (BSF)  $n^+-p-p^+$  structure was under consideration and the influence of the base thickness on ideality factor was taken into account as well.

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