Deep Learning-Based Impurity Evaluation: Targeting Silicon Solar Cells' Photovoltaic Parameters

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***Abstract* — In our work, we applied the deep learning-based approach for estimating am iron concentration in silicon solar cells by using photovoltaic parameters. Different variants of deep neural networks, which involve using either the short-circuit current, photoconversion efficiency, open-circuit voltage, and fill factor values, or only the first two parameters obtained under solar or monochromatic lighting, were examined. The simulation of silicon solar cells for generating labeled datasets was performed using SCAPS-1D software. Networks were tested on synthetic and experimental current-voltage characteristics. It was shown that the mean-squared error of iron concentration predictions can be about 3×10^{-3}. The ways of optimizing the configuration and use of such neural networks are proposed.**

Keywords — silicon solar cell, iron contamination, deep neural network, photovoltaic parameters, SCAPS, recombination centers

I. Introduction

Materials informatics (MI), which combines material property calculations/measurements and informatics algorithms, has become one of the main paradigms of science over the past few years [1]. MI has opened new avenues for accelerating the development, characterization, and investigation of both materials and devices. At the same time, one of the most important directions is the use of machine learning methods, which are focused on solving problems where the possibility of clear algorithm presentation is not foreseen. In particular, similar approaches are widely used in photovoltaics, which occupies a special place among technologies of renewable energy sources. For example, computer-assisted learning is used to identify potentially important photovoltaic materials based on their optical and symmetry properties [2] or the mentions of the various structure names in the literature [3], to predict solar cell current-voltage characteristics (IVC) [4] and their degradation [5] depending on external conditions, and to automate of defect detection procedures based on electroluminescent images [6].

On the other hand, non-destructive methods aimed at estimating the concentration of recombination-active defects, in particular, the impurities, in photovoltaic semiconductor structures are important from an applied point. Today, many direct and indirect methods have been developed to solve this problem. The improvement of methods is often achieved not only by using more advanced experimental procedures and equipment but also due to various mathematical tools. Laplace deep-level transient spectroscopy (LDLTS) [7] may be considered as the most striking example. In this case, the Laplace transforms allowed not only to simplify the experimental procedure compared to classical DLTS (when there are enough measurements at a single temperature) but also a significant increase in the resolution of defects' energy determination.

However, almost all existing methods require special preparation of the research objects or special equipment. At the same time, a simple and generally accepted method of determining the parameters of the photovoltaic conversion of solar cells is the measurement of IVC. Obviously, the presence of recombination centers significantly affects the processes of photoelectric conversion. That means the determination of the characteristics of such defects precisely from the analysis of IVC is both fundamentally possible [8] – [9] and extremely promising for wide use. Obviously, the mathematical tools for IVC processing are perhaps the most important in that case. For example, it was proposed to use differential I-V coefficients [10] and current components [9] for defect characterization. Moreover, the extraction of the current components from measured IV curves is improved by using the Lambert W-function [11]. Lately, the ability to extract the defect parameters from IV measurements and Bayesian parameter estimation utilizing a modified Gaussian likelihood was demonstrated [12]. However, one of the most considerable obstacles to introducing such a convenient and quick method remains the multi-parameter nature of the analytical interrelationship of the recombination center concentration and the IVC features. And it is the use of deep learning methods that can be a way to overcome this obstacle.

In particular, it is about the creation of an artificial deep neural network (DNN), which can predict the concentration of electrically active impurities, using the base general characteristics of a solar cell (SC), measurement conditions, and certain parameters of IVC. Of course, DNN training requires a huge amount of labeled data, and the first step to