On the other hand, non-destructive methods aimed at estimating the concentration of recombination-active defects in photovoltaic semiconductor structures are important from an applied point of view. Many direct and indirect methods have been now developed to solve this problem. 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 current-voltage characteristics (IVCs). Therefore, an express method of impurity determination, which is based on IVC, is very desirable. We have shown the possibility of implementing a similar approach in our previous work (Prog. Photovolt. Res. Appl. 30 (2022), 648). The proposed method used an artificial deep neural network (DNN), and the ideality factor was the parameter sensitive to the influence of recombination centers. However, the accuracy of applying the created network to real SSCs was far from ideal. The reason may be connected to the error in determining the ideality factor from real IVСs and (or) the inaccuracy of the used calculation model.

The plan of research includes constructing a DNN that uses standard photovoltaic parameters: short-circuit current, open-circuit voltage, efficiency, and fill factor. This approach makes it possible to reduce the requirements for IVC measurement. In addition, the measurement of light IVC is a more common way of SCs characterization. The task implementation needs to simulate the IVC of illuminated SSCs to create a training and test data set. The estimated required IVC number is about 100,000, which corresponds to SSC with different parameters and different illumination conditions. During simulation, the latest models for intrinsic recombination and light absorption coefficients in silicon will be taken into account (Solar Energy Materials & Solar Cells **234** (2022) 111428, Solar Energy Materials & Solar Cells **235** (2022) 111467, AIP Advances **5** (2015), 067168). The next step is tuning the architecture and hyperparameters of DNNs to predict iron concentrations in SSCs. Finally, DNN training and testing on artificial and experimental data are needed.

Modern deep learning approaches involve working with big data sets, and requirements for the operation speed and RAM volume of computing devices are rigid. The fellowship would enable to rent of cloud computing resources, which will significantly speed up research.

The second direction provides the construction of an artificial deep neural network (DNN) that estimates iron contamination in SSCs from photovoltaic parameters. The modeling of current-voltage characteristics, DNN tunning, and testing on real SSCs are planned. The proposed approach for impurity estimation uses simple and widely applied equipment and does not take much time.

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. And 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] can be the most striking example. In this case, the Laplace transforms allowed not only to simplify the experimental procedure compared to classical DLTS (the measurements only at a single temperature are enough) but also to significantly increase the resolution of determining the defects' energy.

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 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 а 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 obtain such data can be the SC simulation using standard software. The possibility of implementing a similar approach was shown in our previous work [13], where the dark IVC s were studied, and the ideality factor was considered as the parameter which was essentially sensitive to the influence of recombination centers. This paper presents the results of constructing a DNN that uses standard photovoltaic parameters: short-circuit current (), open-circuit voltage (), efficiency (η), and fill factor (*FF*). This approach makes it possible to reduce the requirements for IVC measurement. In addition, the measurement of light IVC is a more common way of SCs characterization. The choice of monocrystalline silicon photoconverters as a research object is determined by the predominant practical application of such structures. In turn, iron is one of the main and most harmful impurities in such systems, which led to using the DNN for the detection of such recombination centers.

Міністерство освіти на науки

виконавець держбюджетної теми "Дослідження фізичних властивостей емісійних явищ в неоднорідних матеріалах" (№97017)

виконавець держбюджетної теми «Теоретичне та експериментальне дослiдження фiзичних властивостей неоднорiдних систем на основi матерiалiв акусто–опто–електронiки та мiкроелектронiки» (№01БФ051–09)

виконавець держбюджетної теми «Експериментальне та теоретичне дослiдження структури та фiзичних властивостей низькорозмiрних систем на основi напiвпровiдникових структур, рiзних модифiкацiй вуглецю та композитiв» (№0106U006390)

виконавець проєкту УНТЦ "Дослідження та створення методів опто- акустичного контролю матеріалів" (№3555)

виконавець держбюджетної теми «Фундаментальнi дослiдження в галузi фiзики конденсованого стану i елементарних частинок, астрономiї i матерiалознавства для створення основ новiтнiх технологiй» (№0111U004954)

виконавець держбюджетної теми «Формування та фiзичнi властивостi наноструктурованих композитних матерiалiв та функцiональних поверхневих шарiв на основi карбону, напiвпровiдникових та дiелектричних складових» (№0116U004781)

виконавець держбюджетної теми «Розробка фізичних засад функціоналізації наноструктурованих матеріалів на основі карбону, напівпровідникових гетероструктур та поруватого кремнію» (№0119U100303)

науковий керівник проєкту Національного фонду досліджень України «Розробка фізичних засад акусто-керованої модифікації та машинно-орієнтованої характеризації кремнієвих сонячних елементів» (№2020.02/0036)

виконавець держбюджетної теми «Фізико-хімічні властивості наноструктурованих карбон-вмісних та напівпровідникових тонкоплівкових структур для потреб відновлювано-водневої енергетики» (№0122U001953)

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executor of the state budget topic "Experimental and theoretical study of the structure and physical properties of low-dimensional systems based on semiconductor structures, various modifications of carbon, and composites" (No. 0106U006390);

executor of the UNCTC project "Research and development of methods for opto-acoustic monitoring of materials" (No. 3555);

executor of the state budget topic "Fundamental research in the field of condensed matter and elementary particles, astronomy, and materials science for the creation of the foundations of advanced technologies" (No. 0111U004954);

executor of the state budget topic "Formation and physical properties of nanoscale composite materials and functional surface layers based on carbon, semiconductor, and dielectric components" (No. 0116U004781);

executor of the state budget topic "Development of physical principles for the functionalization of nanostructured materials based on carbon, semiconductor heterostructures, and porous silicon" (No. 0119U100303);

scientific supervisor of the project of the National Fund for Research of Ukraine "Development of physical principles of acousto-controlled modification and machine-oriented characterization of silicon solar cells" (No. 2020.02/0036); executor of the state budget topic "Physico-chemical properties of nanostructured carbon-containing and semiconductor thin-film structures for the needs of renewable-hydrogen energy" (No. 0122U001953).