Driving and estimation of iron in silicon solar cell

Renewable energy is vital for modern civilization. And the direct conversion of solar radiation into electricity plays a specific role among various renewable energy technologies. Silicon solar cells (SSCs) constitute 90% of the current global photovoltaic converters production capacity (856 TWh in 2020). These systems are created using amorphous, polycrystalline, or monocrystalline silicon. The c-Si portion is about 84% now. As with other semiconductor devices, SSCs' properties are determined very much by their impurity compositions. As a result, the methods aimed at defect evaluation or modification are significant for practical application.

Iron is the main and one of the most detrimental metallic impurities in SSCs. Frequently, iron-related defects are the main recombination centers that determine the device characteristics in general. In silicon photovoltaics, one of the main methods of impurity deactivation and removing it from the operation zone is gettering Fe atoms at extended defects, oxygen precipitates, or interfaces. The process efficiency depends on the mobility of iron atoms.

Iron atoms in p-Si can be either in an interstitial site or form pairs with an acceptor impurity. In the first case, Fe diffusion capacity is much higher. Therefore, the effective gettering of transition metal atoms requires freeing them from pairs. The light-induced dissociation of the iron-acceptor pairs is known to occur by using intense (> 100 mW/cm^2) illumination with photon energy exceeding the gap. The influence of illumination intensity on the dissociation of iron-boron pairs has already been studied (AIP Advances **3** (2013) 082124; Sol.St.Phen. **242** (2015) 230-235; Phys. Status Solidi A **216** (2019), 1900253; Phys. Status Solidi B **257** (2020), 1900167). However, information about the effect of illumination spectral composition on the dissociation of impurity pairs is absent. On the other hand, the determination of the spectral range corresponding to the most effective iron-boron pairs dissociation will allow optimizing the processes used in the SSCs manufacture and aimed at gettering harmful impurities.

Such spectral range determination is one goal of our research. The efficiency of the light-induced dissociation of Fe-B pairs will be determined from the kinetic of the short-circuit current of SSC. Both monochromatic and broad-spectrum sources will be used to induce the dissociation of iron-boron pairs. Spectrum and radiation intensity calibration of the lights will be carried out. The originality of the proposed approach is related to

i) the use of ready-made solar cells, instead of the initial silicon plates, for researching the processes of decay of iron-acceptor pairs;

ii) the control of the spectral composition of illumination that causes the light-induced pair dissociation.

Our previous investigation revealed that the excitation of acoustic waves in SSC leads to an intensification of iron–boron complex association (J Mater Sci: Mater Electron **33** (2022) 13133). At this stage, it is planned to experimentally investigate the possibility of intensification of light-induced pair dissociation under ultrasound loading conditions. The longitudinal acoustic wave parameters will be varied (in the frequency range of 2-30 MHz and intensity range of 0.1-1 W/cm^2), and optimal parameters value will be determined.

The fellowship will expand the variety of used illumination sources (halogen and xenon lamps; ultraviolet, infrared, and visible laser systems). In addition, the high-power AC generator (frequency of the output signal up to 100 MHz, amplitude up to 100 V, adjustable output resistance, and the possibility of external modulation) is desirable. This purchase will expand the range of used modes of ultrasonic loading.

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 IVCs 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.

In addition, the fellowship will support research performers (including students and postgraduates).