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“Підтримка досліджень провідних та молодих вчених”

Detailed content of the project

Project Title
Development of physical base of both acoustically controlled modification and machine learning-oriented characterization for silicon solar cells

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3. Detailed content of the project
3.1 The current state of the problem (up to 2 pages)

The renewable energy is vital for modern civilization. The direct conversion of solar radiation into electricity plays a special role among various renewable energy technologies. Firstly this approach singularity is deals with ability to meet the energy needs of without chemical and thermal pollution of the environment. Besides the energy generation can directly occur in immediate proximity to consumption. As a result nowadays the solar photovoltaics are the fastest-growing energy technology in the world.

Silicon solar cells (SSCs) are used to produce more than 90% of about 550 GW of energy, which is currently produced by photovoltaic converters. The amorphous, polycrystalline or crystalline silicon is used to such system creation and a last material’s portion is about 40%. Similarly to case of other semiconductor devices, the defect subsystem in general and impurity composition in particular determine the SSC properties predominantly. It should be noted that in purpose to reduce the final cost the low purity crystals are used to SSC manufacturing. So one of the most common as well as the most harmful impurities are atoms of iron and other transition metals. A lot of scientists’ efforts are aimed at a developing and a technological implementing of methods, which must to provide a deactivation of such defects by gettering in particular. But the efficiency of real solar cells is far from the theoretical limit. Therefore it is evident that the issues of understanding the defect behavior and driving of defect state are fundamental to improve the devices performance.

The irradiation and annealing are the well-known methods of semiconductor structure properties driving by activation/deactivation of technologically functional defects. However they affect the whole crystal as well. Another way of defective subsystem modification is the excitation of elastic oscillations in a crystal. In particular, the acoustic waves in non-piezoelectric materials are shown to be able to cause redistribution of impurities and point defects rebuilding. Moreover, this method affect a defect regions selectively and is realized at room temperature. In addition, the ultrasonic loading is shown to be effective additional factor of influence during technological operations, for example, during ion implantation. On the other hand the available information is insufficient to form a holistic view of the acousto-defective interaction in semiconductor crystals and in silicon in particular. As a result, the possibilities of active ultrasound are not used during solar cell manufacturing, unlike to many other technological processes.

Non-destructive methods of estimation of the concentration of impurities (including transition metals) in semiconductor crystals and structures, in particular solar cells, are important from an applied point of view. To date, a not little collection of direct methods (an infrared tomography, an electron-paramagnetic resonance, a non-stationary spectroscopy, etc.) as well as indirect methods (a surface photovoltage, a minority carrier lifetime measurements) has been developed to solve this problem. But almost all of them require either special sample preparing or specialized equipment. At the same time, the current-voltage curve (IVC) measurement is a widespread method of solar cell characterization and allows to determine such fundamental SC parameters as efficiency, open-circuit voltage, and short-circuit current. Evidently these parameters in particular and the processes of carrier propagation in general depend on electrically active defects presence; therefore there is a possibility in principle to determine the defect concentration by IVC shape. One of the main obstacles of such a convenient and express method developing is the multiparameter relationship between the concentration of recombination centers and IVC characteristics, which are determined by experimental curves fitting. However, in the last decade, deep learning, which are enable to solve problems without clear algorithmization, have been successfully used in various fields of theoretical and applied physics. This gives hope for an real implementation of aforesaid SC characterization method with deep learning approaches using.

3.2 The project novelty (up to 1 page)

The first part of the project deals with the experimental establishment of regularities of dynamic acoustically induced effects in SSCs. Unlike to numerous previous studies, where acoustic waves were used as an exclusive tool of irreversible modification of a non-piezoelectric semiconductor by disturbing from a stable (metastable) state, this project is focused on the ascertaining physical features and mechanisms of ultrasound loading influence on the complex point defect rebuilding, which is initiated by another activating factor (lighting) or is caused by the system aspiration for a thermodynamic equilibrium state. That is, the project concentrates effort on the development of the physical principles of the complex method, where ultrasound is regarded as an additional and adjustment factor. In addition, the project novelty is defined by the object of a study of acoustic activity, namely, transition metal atoms and complexes, which involve these atoms, in monocrystalline silicon.

The second part of the project is aimed at developing a new express method of estimating of the recombination centers concentration, which is a simple complement of the standard procedure of SSCs characterization by using IVC. The proposed approach involves a number of new approaches, in particular, the exploitation of the ideality factor value as a quantitative indicator of the recombination centers concentration and the using of deep learning to establish the relationship between aforesaid parameters.

3.3 The research methodology (up to 2 pages)

The project experimental part aims to establish the physical regularities and mechanisms of acoustic waves influence on the rebuilding of defects, which involves transition metal atoms and provides for the following milestones: i) the selection of real SSCs with boron-doped base and high concentration of impurity iron; ii) the determination of influence of light-induced Fe-B pair dissociation on the IVC parameters (an ideality factor, a saturation current, a shunt resistance, an open-circuit voltage, a short-circuit current) of silicon solar cells; iii) the quantification of kinetic of IVC parameters change induced by Fe-B pair association; iv) the finding out of regularities of SSC parameters change, which forced by light-induced degradation, under ultrasonic loading (longitudinal and transverse waves with frequency (1-30) MHz and intensity (0.1-1) W/cm^2 over the temperature range 290-350 K) and the comparison to non-ultrasound case; v) the determination of kinetic characteristics of IVC parameters variation due to Fe-B pair association under ultrasonic loading condition and the comparison to non-ultrasound case; vi) the development of recommendations for targeted changes in SSC performance specification by acoustically stimulated defect deactivation.

The choice of the Fe-B impurity pair as a direct object of acoustically driven modification is defined by several factors. Namely

a) this defect is prevalent in real solar cells and it has a significant impact on the efficiency of photovoltaic conversion;

b) the Fe-B parameters are well-known;

c) this complex are easy to rebuild: pair can be readily dissociated under intense illumination and is repaired in the darkness and the association characteristic time is about tens minutes at room temperature;

d) the pair's components are characterized by crystal volume change $\Delta\Omega$ of different sign: boron is a impurity whose ionic radius is smaller than that of matrix atoms whereas $\Delta\Omega$ for interstitial iron is positive; accordingly to the previous studies such defects are expected to be characterized by highest efficiency of acousto-defect interaction.

The development of the method, which is intended for solar cell impurity characterization and based on the IVC measurement, is provided by modeling of silicon n+-p-p+ structures with transition metal atom impurities (by the example of iron). This part includes numerical simulation of IVC for structures with different base thickness (150-240 μm), base doping level (10^{15}-10^{17} cm^{-3}), impurity concentration (10^{10}-10^{13} cm^{-3}) over the temperature range 290-340 K. The interstitial iron, Fe_iB_s pair and different charge states of the defects would be under consideration. In our numerical simulation we will use of one-dimensional code solar cell simulator SCAPS 3.3.08 and real values and temperature dependences of parameters for silicon and traps (band gap width and narrowing, mobility, carrier thermal velocity and effective mass, intrinsic recombination coefficients, carrier capture cross section, energy level etc.) will be taken into account. The ideality factor determination for the structures under consideration is the next stage. The meta-heuristic optimization method Jaya will be used to IVC non-linear fittings according to the two-diode model. The last stage is tuning (a fitting of numbers of both hidden layer and neuron, regularization method, activation function, learning speed) and training (by using pre-calculated data set) of an artificial neural network, which is able to predict the concentration of impurity iron atoms by utilization of solar cell parameters, measuring conditions and ideality factor value which extracted from IVC. The preliminary tool for neural network driving is the Keras package.

3.4 Justification of the tender participant's ability to implement the project (up to 3 pages).

O. Olikh has a scientific work experience of 24 years, he is the author of more than 70 scientific publications, including 40 articles (10 papers is single author papers in journals, which are Scopus indexed; in particular, 2 and 3 similar works are in the Q1 and Q2 journals, respectively). H-index (Scopus) is equals to 7. His main research subject is using of ultrasound to characterize and modify the properties of semiconductor structures. For the first time he have investigated the charge transfer in silicon p-n and Schottky barrier structures under ultrasound loading conditions; the model of acoustically active complex defect has been proposed by him. O. Olikh is a specialist in determination of barrier structure parameters from IVC, in particular, by using meta-heuristic methods (Journal of Applied Physics, 2015, **118**, 024502). Besides he is the author of a paper, which is base of the proposed in project method and devoted to analyze of relationship between an ideality factor value of silicon n^+-p-structure and the iron concentration (Superlattices and Microstructures, 2019, **136**, 106309).

V. Kostylyov has a scientific work experience of 45 years, he is the author of more than 270 scientific publications, including 1 monograph, 152 articles (54 papers are Scopus indexed; in particular, 4 and 8 works are in the Q1 and Q2 journals, respectively), 6 patents of Ukraine. H-index (Scopus) is equals to 7. His main directions of scientific activity are complex research of electrophysical, photoelectric and optical processes in multilayer photosensitive silicon structures, development of physical and technological principles for creation of new types of photovoltaic devices and solar cells, and development and creation of new methods for investigation mentioned devices and structures. As a research results the features of the generation-recombination processes and the collection of non-equilibrium carriers in silicon structures with near-surface diffusion-field barriers and hetero-transitions (including heterostructures p^+-α-Si:H/n-c-Si/n^+-α-Si:H (HIT)) were clarified over wide temperature and illumination ranges (Journal of Applied Physics, 2016, **119**, 225702; EEE Journal of Photovoltaics, 2020, **10,** 63-69); new mechanism of exciton influence on the charge carrier recombination in silicon due to non-radiative Auger annihilation of excitons with the participation of deep impurity centers is proposed. The obtained results allowed to develop the technology of manufacturing highly efficient silicon converters of solar energy for terrestrial and space purposes with efficiency up to 19% in AM 1.5 conditions. In addition, the physical and technological principles of 30-40% reduction of optical losses in photoconverters by using multilayer anti-reflective coatings and ohmic losses reduction are developed.

Under the framework of the National Space Program of Ukraine, V.P. Kostylyov taken active and creative part in developing and introducing into production of high-performance solar batteries AAEI.564113.001 for new generation spacecraft KS5MF2 "Micron".

V.P. Kostylyov created and headed the only in Ukraine certified Center for testing photoconverters (PC) and photovoltaic batteries (PVB) of the Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine. Center is certified by the Ministry of Economic Development of Ukraine to measure photo-energetic parameters of solar cells and batteries. Center is included in the State Register of scientific objects that are national property (resolution of the Cabinet of Ministers of Ukraine, 28.08.2013 №650-р).

V.P. Kostylov et al. were awarded the State Prize of Ukraine in the field of science and technology in 2013.

V.M. Vlasiuk has a scientific work experience of 5 years, he is the author of 44 scientific publications, including 13 articles (3 papers are in the Q1 and Q2 journals). The research activity is deals with investigation of photoelectric processes in silicon photosensitive structures. For the first time he shown that recombination currents in the space charge region of silicon photosensitive structures have been formed by carriers with very short lifetimes in comparison with volume case. The contribution of non-radiative exciton recombination to the effective lifetime of non-equilibrium charge carriers in silicon is specified. Vlasiuk V.M. is a specialist in determination of photoelectric and recombination parameters of photosensitive structures.

O. Lozitsky has a scientific work experience of 4 years, he is post-graduate student. He is the author of 14 papers (12 are Scopus indexed and 6 are in the Q1 and Q2 journals). H-index (Scopus) is equals to 3. O. Lozytsky is experienced in modeling of physical properties of material by using machine learning. Particularly, the shielding and electrical properties of single- and multilayer composites in the microwave range were modeled by him. There is also experience in using reinforcement learning on the Upwork platform.

Center of PC and PVB testing is equipped by the following equipment and standard samples:

- the setup of phototechnical tests of solar cells;
- the setup of determination of spectral characteristics of photoconverters;
- the setup of electrical and phototechnical tests of solar panels;
- the measuring device for photoenergy parameters of solar modules "Photon-3";
- the setup of pulse testing of photovoltaic modules and batteries;
- the measuring device for energy lighting BEO-01;
- the standard photoconvertors;
- the laser ellipsometer.

In addition, the available material and technical resources includes the following elements

- the setup of current-voltage characteristic measuring ((-5-5) V, (10^{-8}-$2\cdot10^{-2}$) A, accuracy 0,1%, working rate – up to 50 measurement/s);
- the thermostat with proportional-integral-differential controller (temperature stability ±0,02 K);
- the piezoelectric transducers for excitation of longitudinal and transverse waves (1-30 MHz);
- the complex for ultrasound loading (generator Г3-41, wavemeter Ч3-34, digital oscilloscope GDS-806S, characterograph Х1-48);
- PC AMDA4–3400, 2.7GHz CPU, 3072 MB RAM.

3.5 The substantiation of the need to equipment purchase by the grant expense and the directions of equipment use after the grant ending (up to 1 page).

The grant provides for the purchase of the following equipment:

- Keithley 4200A-SCS Parameter Analyzer with units Keithley 4200-SMU, Keithley 4210-CVU and Keithley 4200A-CVIV. This device allows to carry out with high accuracy fast measurements of current-voltage characteristics (current range 10^{-15}-1 A, voltage range 10^{-6}-210 V) and capacity-voltage characteristics (10^{-14}-10^{-6} F, up to 400 V, frequency range 10^{3}-10^{7} MHz).

The purchase necessity is determined by following reasons. 1) The high-speed IVC measurements are possible: Keithley 4200A-SCS separation time reaches 10 ns in pulse mode and significantly exceeds the capabilities of existing equipment; at the same time, the characteristic time of the rebuilding and recharging of defects in semiconductor devices is often in the range of 10^{-6}-10^{-2} s and therefore this device will enabled the direct determination of physical features for such processes and the impact of acoustic waves; 2) The capacity-voltage measurement ability leads to expanding possibility SSC testing and preparation of recommendations for the modification of technological processes. After project finalization, the Keithley 4200A-SCS Parameter Analyzer will be used to test a variety of semiconductor devices and structures. In particular, the possibility of ultra-fast small current measurements allows to characterize nanoelectronic devices.

- Laptop HP Pavilion Gaming 15. Modern deep learning approaches involve working with big data sets, therefore requirements for the operation speed and RAM volume of computing devices are rigid. In particular, parallel computing processes using video processors with CUDA technology support are widely used. Most of the present artificial neural networks tools (in particular, Keras, which is planned to be used during the project) are optimized to similar technologies using. Unfortunately, the existing PC set is outdated from this point of view and effective work with an artificial neural network, which is able to predict an impurity concentration by solar cell parameters, requires equipment with more computing power. After project finalization, the laptop will continue to be used to implement deep learning processes.

3.6 The amount of funding required to carry out the research (development), with the appropriate justification for the cost items according to the tables in Section VII (up to 2 pages).

The total labour compensation expenses provide funding in the amount of 1886210 uah (390250 uah 1st year, 1495960 uah 2nd year). They are planned in accordance with the salary scheme of the Taras Shevchenko National University of Kyiv and project executor works are listed in the following table.

Name	Tasks	Employment, month
Olikh O.Ya., doctor of science, assoc. prof., project scientific head	Development of a calculation model of silicon n+-p-p+ structure; development of software for automation of modeling and results processing; numerical calculation; development of procedure for quantification of kinetic of IVC parameters change under ultrasound loading; development of methods for extracting parameters from IVCs; development of artificial neural network architecture; determination of mechanisms of acousto-defective interaction; development of recommendations for the method of quantitative evaluation of electrically active defects in barrier structures by the ideality factor value; writing of presentations, papers, and reports	14,5
Kostylov V.P. doctor of science, prof.	The selection of silicon solar cells; development of procedure for measuring of kinetics of light-induced processes in SSCs; quantification of kinetic of IVC parameters changes due to Fe-B pair association; determination of mechanisms of acoustic wave influence defect complex rebuilding; development of recommendations about using of ultrasound loading during SSC manufacturing; writing of presentations, papers, and reports	14,5
Vlasiuk V.M., PhD	Equipment purchase; testing of modes for measuring of kinetics of light-induced processes in SSCs; measuring of influence of light-induced dissociation of Fe-B pairs on the IVC parameters both with and without ultrasound loading; writing of presentations, papers, and reports	14,5
Lozitsky O.V., post-graduate student	Development of software for automation of modeling and results processing; numerical calculation; software implementation of the meta-heuristic optimization method Jaya; tuning and training of an artificial neural network; writing of presentations, papers, and reports	14,5
young scientist, PhD	Practical implementations of procedure for quantification of kinetic of IVC parameters change under ultrasound loading; measurements of kinetic of IVC parameters change.	8,5
young scientist, post-graduate student	Measurements of characteristics of IVC parameters changes due to Fe-B pair association both with and without ultrasound loading; equipment purchase	8,5
student	Practical implementations of procedure for quantification of kinetic of IVC parameters change under ultrasound loading; sample preparation	8,5

Funding for materials needed to perform the work, in addition to special equipment is 166900 uah (65000 uah 1st year, 101900 uah 2nd year). Preferably, it involves the cost of components required for the parametric analyzer Keithley 4200A-SCS operation. In addition, purchase of paper and consumables for printers is planned due to report prepare need (7110 uah).

The equipment expenses are 3368370 uah (2262620 uah 1st year, 1105750 uah 2nd year); the justification is given in 3.5.

Business trip expenses are related to the need to present the scientific results as well as to get acquainted with the latest achievements. It is provided 4 business trip abroad and 2 business trip internal, the total expenses – 179330 uah (2nd year).

Other expenses 257140 uah (2nd year) are intended for the payment of publication fees (2 papers, which are provided in the project expected results) and organizational fees at scientific conferences.

The total project expenses equal to 6508830 uah (3019860 uah 1st year, 3488970 uah 2nd year)

3.7 The project’s expected results (up to 1 page):

The expected project scientific products are following:
- the finding out the physical regularities and mechanisms of interaction between ultrasound waves and defect complexes, which associated with transition metal atoms;
- the evaluation of possibility of targeted changes in SSC performance by using ultrasound during manufacturing and development of recommendations for the practical using;
- the development of physical base of method for estimation of concentration of electrically active defects in barrier structures by an ideality factor value;
- the creation of data array (about 15 000 sets) of calculated ideality factor value for silicon n^+-p-p^+ structures with various geometric and electrophysical characteristics;
- the tuning of an artificial neural network to estimate the concentration of iron atoms in silicon n^+-p-p^+ structures
- at least 2 papers in Q1 and Q2 journals;
- at least 3 presentation at international conference.

3.8 The ways and means of further use of project implementation results in public practice (up to 1 page).

The established physical regularities of the ultrasonic loading influence on the rebuilding of defect complexes, which associated with transition metal atoms, can be used to modify the standard technological operations of silicon solar cell manufacturing to deactivate these defects. The determined features of the acousto-defect interaction will allow to adjust the ultrasound parameters to raise efficiency of the controlled modification of the defective subsystem. In addition, the results can be the basis for the development of methods of acoustic engineering of defects in semiconductor devices.

The established quantitative relationship between an ideality factor value and the concentration of recombination centers can be used as a basis for the express method of estimating the impurity composition of real solar cells. The tuned artificial neural network can be directly used to estimate the concentration of iron atoms in silicon n^+-p-p^+ structures, where these defects are the main recombination centers.

3.9 Possible risks, which may affect the project implementation (up to 1 page)

The quarantine will prevent the full implementation of experimental research.