ABSTRACT

dissertations for the degree of doctor of philosophy (PhD) in the specialty
6D072300 – «Technical physics»
(by industry)

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Study and optimization of silicon-based heterojunction solar cells

The scientific work presents the results of changes in the technological parameters of the formation of structures of heterojunction solar cells of computer simulation, as well as experimental studies of the physical properties and structures of GIT solar cells.

Relevance of the research. Already established in the minds of people, as the most common in the market of crystalline solar cells, in which p-n – transition is obtained by diffusion, have advantages such as a relatively high efficiency and technological maturity. At the same time, the disadvantage of such solar cells is the relatively high cost of production associated with the need to use high temperatures up to 1000°C, as well as the requirement for high purity of crystalline silicon to obtain high efficiency. Amorphous silicon is one of the cheapest alternative materials for solar energy, but the maximum efficiency of laboratory solar cells from it reaches only 13.4%. Amorphous and crystalline silicon have different optoelectronic properties, wider-band amorphous silicon (Eg = 1.9 eV compared to Eg = 1.12 eV crystalline silicon) has a higher optical absorption coefficient of light in the visible spectrum. Combining the advantages of the two materials to create a hetero-junction solar cell, known as «HIT» (hetero-junction with intrinsic thin layer), demonstrates the ability to achieve high solar energy conversion efficiency of about 25% when using less silicon and lower manufacturing process temperatures not exceeding 200-250°C. On an industrial scale, the technology of silicon hetero-junction makes it possible to obtain solar cells with an efficiency of more than 18%.

The technology of heterojunction silicon solar cells was first patented by Sanyo in the early 1990s. In the initial cells described by Tanaka and colleagues, the heterojunction was formed on the basis of a smooth crystalline silicon (c-Si) plate of n-type, on the surface of which a thin layer of amorphous hydrogenated silicon (a-Si:H) of p-type conductivity was deposited . The maximum value of the efficiency coefficient for such a solar cell structure reached 12.3%, while the maximum efficiency was obtained for the thickness of the amorphous layer of the order of 100 Å (10 nm). It was also found that the introduction of a thin film a-Si:H of intrinsic conductivity between silicon layers of n-and p-type allows to reduce the density of surface defects at the interface between crystalline and amorphous silicon, this is reflected simultaneously on the increase in the no-load voltage, short-circuit current and the solar cell fill factor. In this case, the efficiency increased to 14.8%, while the optimal thickness of the amorphous silicon layer of intrinsic conductivity was 60-70 Å. Another innovation of Sanyo was the creation of a textured surface of the solar cell for more efficient absorption of light, as well as the ability to absorb light falling on the plate at small angles. No texturing conditions were specified, but it was mentioned that the crystal plate was subjected to plasma treatment in hydrogen prior to deposition of a-Si:H. In addition, to create an electric field on the back side of the solar cell, a layer of a-Si:H n-type conductivity was deposited on the reverse side of the silicon plate. As a result, the efficiency of the solar cell reached 18.1% for a sample size of 1 cm^2.

In recent years, more and more works have been devoted to the study of HIT solar cells, however, there are not so many experimental works. For the most part, leaders in the field of HIT technology report the use of cleaner and more expensive materials to achieve high efficiency solar cells in the laboratory. The works devoted to the modification of the design of HIT photocells are mainly based on the use of computer simulation, but for the most part, they do not consider the HIT photocell as a whole, only some individual parts of it. It is worth noting that there is a problem of improving the quality of HIT structure photocells in an industrial environment, and this issue is mainly considered from the side of optimization of technological processes and equipment operating modes, but not from the side of improving a photocell structure design.

A comprehensive approach to optimizing the technological parameters of the HIT structure using computer simulation methods, theoretical and numerical calculations, as well as experimental studies using industrial or semi-industrial equipment, can serve as a solution to the problem of improving the quality of solar cells in an industrial environment.

The aim of the work is to optimize the technological parameters of the formation of the structure of heterojunction solar cells to achieve their efficiency of 20% or more.

To achieve this goal the following **tasks** were solved:

1) To study the standard technology for the production of heterojunction silicon solar cells and to develop a method for its improvement.

2) Using computer simulation using the AFORS-HET software package, determine the parameters that affect the efficiency of heterojunction silicon solar cells.

3) To optimize the computer model of the HIT photocell with theoretical calculations based on the physical laws of semiconductor electronics and photovoltaics.

4) To carry out experiments for optimization of the technological parameters of the photocell HIT structure, in particular, the thickness of: the emitter layer in solar cell integrated front layer of intrinsic conductivity in solar cell integrated back sheet intrinsic conduction in the solar cell, BSF layer.

5) To produce optimized experimental HIT prototypes with an efficiency of more than 20% and investigate their characteristics by measuring optical and IV characteristics.

Object of research. Heterojunction photovoltaic cells with a built-in thin amorphous layer based on a monocrystalline silicon substrate of n-type conductivity.

Subject of research. Technological parameters of the structure of heterojunction solar cells HIT.

Scientific and practical significance of research.

- The possibility of optimizing the technological parameters of the structure of solar cells through computer simulation, using the algorithm presented in the paper.

- The optimal values of the characteristics of HIT FEP, which can be used in the industrial production of solar cells.

Scientific novelty the following results have:

1) For the first time using an integrated approach that includes experimental studies, theoretical calculations and computer modeling, the optimal geometric parameters and doping levels of functional layers are found that affect the output characteristics of the studied HIT photocell.

2) For an HIT photocell manufactured under industrial conditions on the basis of a commercial n-type single crystal wafer, the optimum thickness of the emitter amorphous p-type conductivity layer was determined.

3) For a HIT photocell manufactured under industrial conditions on the basis of a commercial n-type single crystal wafer, the optimal thickness values were first determined for the front and back embedded amorphous intrinsic layers.

4) On HIT heterojunction solar cells manufactured under industrial conditions using optimal technological parameters of the structure, an efficiency of more than 20% is achieved.

Scientific provisions submitted for protection:

1) The structure of p-a-Si:H / i-a-Si:H / n-c-Si / i-a-Si:H/ n+ a-Si:H optimized on the basis of the developed method has the following optimal technological parameters: thickness of the p-a-Si: H – layer, frontal The i-a-Si: H – layer, the n-c-Si layer and the back i-a-Si: H – layer are 7 nm, 5–7 nm, 200 μm and 7–11 nm, respectively.

2) The efficiency of HIT photocells based on a single-crystal plate of the n type conductivity depends on the thickness of the emitter p layer so that its optimal experimental value is 10 nm, and a further increase in the thickness is accompanied by a decrease in the short-circuit current and a decrease in efficiency. A decrease in the p-layer thickness leads to an increase in the short circuit current of the photocell, which occurs up to a p-layer thickness of 8 nm.

3) The efficiency of HIT photocells based on an n-type single crystal plate depends on the thickness of the front and back layers of amorphous silicon of the i-type so that their optimal experimental values are 7 and 9 nm, respectively, and their further increase leads to a decrease in open circuit voltage and values Efficiency.

4) The value of the efficiency of HIT photocells optimized on the basis of computer simulation data, theoretical calculations and experimental results is more than 20 percent.

General characteristics of the work.

Significant achievements in photovoltaics recently contributed to a strong fundamental understanding of the properties of materials and the ability to finetune their structure using modeling methods. Among the most widely used and easily accessible packages are AFORS-HET and PC1D. Earlier studies using these tools focused on the influence on the characteristics of the device of the electrode functions and their doping density, the introduction of p + back layer in the heterojunction, as well as the role of the position of the Fermi level in the doped, a-Si: H and displacements at the a-Si: H / c-Si boundary.

To determine the main factors affecting their efficiency, solar cell modeling was carried out using the software packages "PC1D" and "AFORS-HET". In particular, both standard solar cells based on crystalline silicon and amorphous silicon solar cells and elements based on the "amorphous silicon - crystalline silicon"heterojunction were simulated. The thesis demonstrates an approach in which the search for thin measuring ranges in the layer thickness and doping in multilayer solar cells is carried out using simpler systems.

Based on the results of modeling using simplified structures of solar cells, it is possible to evaluate and evaluate the level of influence of each of the manufacturing parameters on the efficiency of the more complex solar cell HIT.

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Using an approximate system of highly efficient heterojunction silicon solar cell, the optimal algorithm for solar cell optimization using the AFORS-HET modeling tool is found. Initially, we identified the relative effects of changes in each of the device parameters, in particular, the thickness and doping levels for each layer. This was done by looking at simpler device structures containing certain elements of the HIT structure. Then we estimated these parameters due to their influence on the efficiency of power conversion of the device. Eventually optimized the standard solar cell HIT using three different optimization step sequences: ascending order, descending order and random order. It is demonstrated that different optimization sequences lead to different final parameters of the device and their performance characteristics, and the order of decreasing optimization steps demonstrates higher efficiency than ascending and random orders.

Presents an approach to optimize the cells HIT on the basis of descending order, compared with optimization using the inverse, increasing the order of the steps of optimization and randomization of optimization steps. It was found that although the range of values used for the parameters used in the optimization approaches were the same, the order of decreasing optimization steps resulted in higher efficiency efficiency of 21.02% compared to 20.78% for increasing and 20.49% for random optimization order. The presented approach can be applied in the optimization of other types of solar cells with many optimization parameters, for example, such as multi-pass and cascade solar cells, both in simulation and in laboratory studies.

The solar cell of the HIT structure was modeled in the program AFORS-HET, and then optimized by the author's method. Also in the method optimization was included, additional analyses of the heterojunction between layers of solar cells according to the Anderson model. In addition, experimental results on the passivation of defects on the surface of silicon monocrystalline plates by applying a layer of thin amorphous hydrogenated silicon of its own type of conductivity were taken into account. A computer-optimized model of the solar cell was shown in the aggregate of computer optimization data and additional calculations, as well as taking into account experimental data on silicon passivation. It was found that the optimal parameters of the functional layers of the HIT structure photocell:

- the thickness of the amorphous layer of the p type conductivity is 7 nm, and the level of doping with impurities is of the order of 1020 cm-3;
- the thickness of the substrate of crystalline silicon of the n type conductivity is 200 μm, the degree of doping with impurities depends on the parameters of the crystal plate itself, in the samples under study a value of the order of 1017 cm-3;
- the thickness of the amorphous layer of the n type conductivity can take any value that provides the necessary energy barrier for minority charge carriers, the optimal level of doping with impurities should be of the order of 1020 cm-3.
- It is shown that with an increase in the thickness of the built-in layer of amorphous silicon of intrinsic conductivity, the number of surface defects decreases, but the structure resistance increases. The optimal thickness for the front layer of intrinsic conductivity is 5–7 nm. For the back layer of intrinsic conductivity, the optimum thickness is in the range of 7–11 nm.

A parallel stage was used to study the structure on real samples. To carry out the experiments, photovoltaic cells of the HIT structure with different parameters were made, which were compared in the future by various parameters: the thickness of the amorphous silicon layers of intrinsic conductivity, both from the back and from the front side; the thickness of the p-type layers of conductivity from the front side of the solar cell; the thickness of the back BSF layers of amorphous silicon of n-type conductivity.

One of the most important design elements in solid-state solar cells is the p-n or p-i-n junction, in which the electric charge is generated under the action of sunlight. In this paper, a commercial crystalline silicon wafer was used as the n-layer, and the i - and p - layers were sprayed by plasma chemical gas deposition (PECVD). The method consists in decomposition of reaction gases into radicals by means of gas-discharge plasma. Then there is the deposition of radicals on the surface of the substrate. During the deposition process, the substrate is on a heated holder, where the temperature is maintained at 2000C. A high-frequency voltage is applied to the electrodes in the chamber, which is filled with reaction and accompanying gases. After the ignition of the capacitive discharge, the gas mixture decomposes into electrons, ions and radicals. Further, ions and radicals are deposited on the substrate, where the growth of the amorphous film occurs.

After manufacturing the samples, electrical properties were measured. Measuring the current-voltage characteristics (I-V) and quantum efficiency are made on the installation of "IV-16 L".

Hetero-junction solar elements of the HIT structure with different parameters were investigated. The analysis of such characteristics of manufactured solar cells as no-load voltage, short-circuit current, form factor and efficiency.

It was found that the effect of reducing the thickness of the p-layer is to increase the short-circuit current. The current increase continues up to the p-layer thickness of 8 nm and then decreases. In addition to increasing the short-circuit current, reducing the thickness of the p-layer reduces the no-load voltage and form factor. The decrease in the no-load voltage is due to the recombination of charge carriers in the structure. The influence of all these factors leads to the fact that the maximum efficiency of the solar cells is observed at a p-layer thickness of 10 nm.

During the experiment it was shown that the optimal thickness of the n-layer may differ for different plates.

It is shown that the optimal thickness of the frontal i-a-Si:H layer is 7 nm, while the optimal value for the back layer i-a-Si:H is 9 nm. This is due to the influence of the amorphous film on the no-load voltage, which may be due to a change in the probability of recombination of charge carriers in the structure.

On site Ioffe Institute during foreign internships mastered the technology of production of solar cells structure of the HIT solar cells is made of the above-described structure. The best optimized solar cells had an efficiency of more than 20%.

The methodological basis of the research is the methods of obtaining multilayer hetero-structural silicon solar cells with a built-in thin buffer amorphous layer and methods for measuring the electrical and optical characteristics of the produced elements. Also, one of the research methods is computer modeling and numerical methods for calculating the computer model, analytical methods for calculating the hetero-junction.

Use of the research. The main results of the dissertation work reported and discussed at the following conferences and seminars:

1. 2016. «Science and Applications of Thin Films, Conference & Exhibition (SATF 2016)», Izmir, Turkey.
2. 2016. «Amorphous and microcrystalline semiconductors», St. Petersburg, Russia.
3. 2017. «New materials and technologies: powder metallurgy, composite materials, protective coatings, additive technologies and robotics», Almaty, Kazakhstan.
4. 2017. «Physical and chemical problems of renewable energy», St. Petersburg, Russia.
5. 2017. «19 all-Russian youth conference on physics of semiconductors and nanostructures, opto-and nanoelectronics», St. Petersburg, Russia.
6. 2018. International scientific conference of students and young scientists «FARABI ALEMI» Almaty, Kazakhstan.
7. 2018. International scientific and practical conference «Global science and innovation 2018», Astana, Kazakhstan.

Volume and structure of the thesis. The thesis consists of an introduction, four sections, conclusion and a list of references containing 119 titles. The work is presented on 110 pages of typewritten text, including 54 figures and 18 tables.