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Computer simulation of amorphous silicon thin-film solar cell with embedded coaxial junction nanowires

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Abstract. This work studies a thin-film amorphous Si solar cell with a coaxial *p-i-n* structure in the form of a nanowire with vertically oriented *p-n* junctions embedded into the structure of a planar basic solar cell with traditional horizontal *p-n* junction. A three-dimensional model of the solar cell is built using the Silvaco TCAD software package and its basic electrical characteristics are obtained. It is shown that the considered design of solar cell allows a significant increase of the photoconversion efficiency at oblique sunlight incidence.

Keywords: solar cell, amorphous silicon, Silvaco TCAD, *I–V* characteristics, solar cell efficiency.

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1. Introduction

Use of thin-film amorphous Si solar cells in the solar energy industry creates problems related to the relatively low efficiency of photoelectric conversion. Increasing the ability to absorb light in thin-film solar cells with a low probability of absorption in a thin semiconductor layer becomes one of the main problems, to overcome which developers offer various design and technological solutions. Thin-film solar cells typically require use of special structures or technologies to capture and retain solar light in order to enhance light absorption and improve the overall efficiency. Such structures are designed to increase the photon optical path length of incident light inside the solar cell, thus increasing the chances of light to be absorbed and reducing reflection losses.

One promising way to increase interaction of solar radiation with a semiconductor material by improving retention and absorption of light in the photoactive layers of a thin-film solar cell is the use of nanoscale structures, such as metal nanoparticles, nanowires, quantum dots, and others [1, 2]. Recently, methods of increasing the efficiency of thin-film solar cells using such nanostructures as nanowires have attracted considerable attention. Nanowires are solid semiconductor nanostructures with diameters in the nanometer range and lengths from a few hundred nanometers to a few micrometers. Nanowires have high surface-to-volume ratios, which allows for more efficient light trapping and absorption. The incident light can be scattered multiple times in the nanowire array, increasing the optical path length and absorption probability. This enhanced light absorption is particularly useful for thin-film solar cells with short diffusion lengths of charge carriers or for the wavelengths that are inefficiently absorbed by the active material. Nanowires can be embedded directly into the photoactive layer of a solar cell or used as textured interfaces between photoactive layers to improve light trapping and absorption.

Coaxial (radial) nanowires in the form of *p-i-n* structures with radial *p-n* junctions, which provide higher efficiency as compared to axial *p-i-n* nanowire structures, have recently attracted great attention of researchers. In such solar cells, charge carriers move along the nanowire radius, covering a short distance not exceeding the diffusion length of minority charge carriers. This minimizes the probability of recombination in the semiconductor layer. Instead, the light passes along the nanowire, which provides excellent conditions for interaction of the radiation with the semiconductor material [3]. Thus, in nanowire-based solar cells, orthogonalization of the directions, along which photons and charge carriers move, is implemented, which allows one to optimize the structure of the solar cell for more efficient light absorption and charge collection independently. This property of coaxial *p-i-n* nanowire structures makes them similar to solar cells with vertical *p-n* junctions. Better charge collection capabilities, while maintaining efficient photon absorption in coaxial nanowires, make it possible to use a lower-quality semiconductor material in smaller quantities to achieve the desired photoelectric conversion efficiency, which results in substantial reduction of the manufacturing cost.

The advantages of solar cells based on nanowire arrays with radial *p-n* junctions and the prospects for further research and improvement of such structures of photovoltaic converters are analyzed in the review works [4-6]. Methods and problems of manufacturing solar cells based on nanowires with radial charge transition are covered in [7]. Many works have been devoted to solving the problem of increasing efficiency of solar cells based on nanoscale coaxial *p-i-n* structures. The efficiency of a solar cell based on amorphous Si coaxial *p-i-n* structures, into which Al-doped ZnO nanowires are embedded, is analyzed in [8]. It is shown that such a coaxial structure provides a 46% increase in efficiency compared to conventional amorphous Si solar cells. Light-retaining properties of solar cells made of Si nanowires are studied in [9]. In this work, a significant increase in the path length of photons in the nanowire array is demonstrated.

The radial *p-i-n* structure of a nanowire is quite difficult for computer modeling because it requires constructing three-dimensional models or use of appropriate modeling tools. A rigorous finite-difference time-domain method together with experimental verification of the calculation results was applied in [10] to determine optical and photovoltaic properties of solar cells based on Si nanowires with radial *p-n* junctions. A 7% photoelectric conversion efficiency was obtained. The finite element method was applied in [11] to model solar cells made of horizontally arranged Si nanowires with axial or radial *p-n* junctions, and the advantages of the radial junction arrangement were demonstrated. An analytical model based on the Green’s functions theory was developed in [12] for simulating Si solar cells in the form of nanowires with radial *p-n* junctions. It was shown that such a model, although having certain limitations, made it possible to find a solution of Poisson and continuity equations and to determine the solar cell basic electrical characteristics.

A Comsol Multiphysics software package was used in [13] to simulate a vertically oriented Si nanowire with a radial *p-n* junction. An 8.2% photoelectric conversion efficiency was obtained at room temperature. This package was also used in [14] for a detailed simulation of light propagation and absorption processes in a complex coaxial multilayer structure of a thin-film amorphous Si solar cell. In [15], the effect of temperature on the *I-V* characteristics of a coaxial *p-i-n* structure in the form of a nanowire based on indium phosphide was investigated using a TCAD software package. Greater thermal stability of the electrical characteristics of direct band semiconductor materials compared to indirect band semiconductors was shown.

This study presents the results of computer modeling of a solar cell structure formed by embedding a nanowire with a vertically oriented coaxial *p-n* junction into a planar thin-film amorphous Si solar cell with a horizontal *p-n* junction. Such an integrated design may be considered as a tandem solar cell with additional options for optimizing parameters to combine the advantages of both a coaxial nanowire and a conventional planar *p-i-n* structure of a thin-film photoelectric converter in one solar cell structure. The main attention is focused on the study of the influence of oblique incidence of solar radiation on the solar cell photovoltaic characteristics. It is shown that the considered design has advantages over a classical planar thin-film solar cell structure at oblique sunlight incidence. Therefore, it may be used on the surfaces hardly lit by orthogonal irradiation, such as on the side surfaces of buildings and vehicles.

2. Solar cell structure and simulation techniques

The design of a photoelectric converter considered in this study is a traditional thin-film amorphous Si solar cell, the illuminated surface of which contains vertically oriented nanowires structurally integrated with the basic horizontal solar cell. The nanowires form a regular grid on the illuminated surface of the basic solar cell to effectively trap solar radiation and significantly increase the photoactive area especially at oblique sunlight incidence. Since such a structure is quite complicated to model, it is reasonable to consider a model limited to one nanowire and a certain region of the basic solar cell, the area of which corresponds to the nanowires density in the array. Under the conditions when the nanowires do not significantly affect each other (no mutual shading), the obtained results may be generalized to a complete solar cell structure. The solar cell structure under consideration was simulated using a Silvaco TCAD software package [16, 17]. Three-dimensional model of the studied solar cell is shown in Fig. 1. Fig. 2 shows a cross-sectional side view of the solar cell structure.

The solar cell model consists of a basic *p-i-n* structure with a traditional horizontal *p-n* junction and a nanowire formed by a coaxial *p-i-n* structure with vertical orientation of *p-n* junctions. The basic structure and the nanowire have a combined low-doped amorphous Si absorber layer, high-doped diffusion layers, and transparent indium tin oxide (ITO) electrodes. Thus, the coaxial *p-i-n* structure of the nanowire is integrated into the structure of the basic solar cell. The thickness of the lightly doped absorbing layer of the *p-i-n* structure is 36 nm, and the thicknesses of the diffuse highly doped *n*- and *p*-type layers are 15 nm and 25 nm, respectively. The concentration of the donor impurity in the absorbing layer is 10^{14} cm^{-3}. The impurity concentration in the *n*- and *p*-type diffuse layers is 10^{18} and $2\cdot10^{17}$ cm^{-3}, respectively. The parameters of the planar *p-i-n* structure of the basic solar cell and the coaxial *p-i-n* structure of the nanowire are matched. Indium tin oxide electrodes are 5 nm thick.

The intensity of solar radiation to determine the generation coefficient was calculated within the framework of the geometric optics approximation (ray tracing method) under AM1.5 standard atmospheric conditions. It should be noted that for nanoscale structures, it is more adequate to use rigorous electrodynamic finite-difference time-domain (FDTD) method.

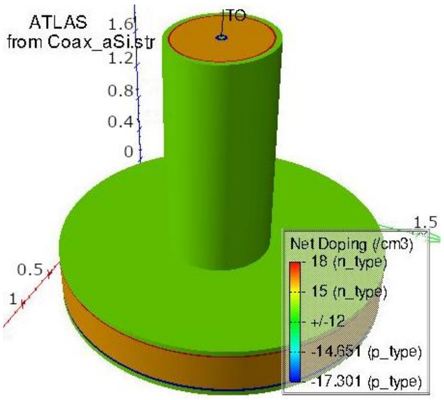

Fig. 1. 3-D view of the solar cell structure.

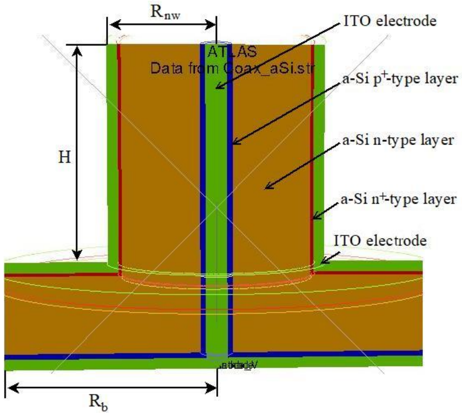

Fig. 2. Cross-sectional view of the solar cell structure.

However, 3D modeling with Silvaco TCAD has significant limitations. Only geometric optics approach can be used to determine the radiation intensity when modeling three-dimensional semiconductor structures. Moreover, periodic boundary conditions cannot be applied. This makes it impossible to consider this solar cell structure as a periodic array of nanowires integrated into a planar solar cell. It is also not possible to use two different coordinate systems in the same model. Therefore, the model of the solar cell includes one nanowire with a section of the basic planar solar cell, also of a radial shape. Such model limitations do not affect the simulation results unless the conditions under which mutual influence of nanowires in the array becomes significant are set.

Silvaco TCAD has a component ATLAS to determine electrical characteristics of semiconductor devices. This component can simulate physical processes in semiconductor structures using different charge transfer models. In this research, the drift-diffusion transfer model was chosen, which adequately describes physical processes in semiconductor devices and was successfully used in earlier works [18, 19]. The mathematical model used in ATLAS to analyze the electrical characteristics of semiconductor devices is a system of fundamental equations that relate the electrostatic potential and current density within a given region. These equations include Poisson equations, continuity equations, and transport equations [17].

The Poisson equation relates the electrostatic potential to the space charge density:

$$\operatorname{div}(\varepsilon\nabla\psi) = -\rho, \tag{1}$$

where ψ is the electrostatic potential, ε is the local dielectric permittivity, and ρ is the local space charge density, respectively. The electric field is defined as the gradient of the potential:

$$\vec{E} = -\nabla\psi. \tag{2}$$

The continuity equations for electrons and holes are given by the following relations:

$$\begin{aligned} \frac{\partial n}{\partial t} &= \frac{1}{q}\operatorname{div}\vec{J}_n + G_n - R_n, \\ \frac{\partial p}{\partial t} &= -\frac{1}{q}\operatorname{div}\vec{J}_p + G_p - R_p, \end{aligned} \tag{3}$$

where n and p are the concentrations of electrons and holes, respectively, $\vec{J}_n$ and $\vec{J}_p$ are the densities of the electron and hole currents, G_n and G_p are the electron and hole generation rates, R_n and R_p are electron and hole recombination rates, and q is the electron charge magnitude, respectively.

According to the drift-diffusion transfer model, the transport equations are formulated as follows:

$$\begin{aligned} \vec{J}_n &= qn\mu_n\vec{E}_n + qD_n\nabla n, \\ \vec{J}_p &= qp\mu_p\vec{E}_p - qD_p\nabla p, \end{aligned} \tag{4}$$

where μ_n and μ_p are the electron and hole mobilities dependent on the carrier concentration, $\vec{E}_n$ and $\vec{E}_p$ are the effective electric fields for electrons and holes, and D_n and D_p are the electron and hole diffusion coefficients, respectively.

$\vec{E}_n$ and $\vec{E}_p$ in the transport equations are the effective electric fields for electrons and holes calculated by the following expressions:

$$\begin{aligned} \vec{E}_n &= -\nabla\left(\psi + \frac{kT_L}{q}\ln n_{ie}\right) \\ \vec{E}_p &= -\nabla\left(\psi - \frac{kT_L}{q}\ln n_{ie}\right), \end{aligned} \tag{5}$$

where T_L is the lattice absolute temperature and n_{ie} is the effective intrinsic concentration of charge carriers obtained from empirical formulas.

D_n and D_p in the transport equations are the diffusion coefficients of electrons and holes, which are determined from Einstein's relations in terms of Boltzmann statistics as follows:

$$\begin{aligned} D_n &= \frac{kT_L}{q}\mu_n, \\ D_p &= \frac{kT_L}{q}\mu_p. \end{aligned} \tag{6}$$

The recombination processes are described in the framework of the Shockley–Read–Hall and Auger recombination models which take into account the doping levels:

$$R(p,n) = \frac{pn - n_{ie}^2}{\tau_p (p + n_{ie}) / [1 + N_\Sigma / N_0] + \tau_n (n + n_{ie}) / [1 + N_\Sigma / N_0]} . \tag{7}$$

Here, τ_p and τ_n are the lifetime of charge carriers specified by the user and depending on the quality of the semiconductor material, and N_Σ is the total concentration of donors and acceptors, respectively.

The advantage of the drift-diffusion transfer model is that it does not use other independent values except ψ, n and p. To determine values of these three independent variables, it is necessary to solve a system of three coupled nonlinear partial differential equations. For this purpose, the area occupied by the semiconductor structure is divided by a 3-D coordinate grid, at the nodes of which all the quantities to be determined are calculated. The coordinate grid used for calculations is shown in Fig. 3 for the cross-sectional side view of the solar cell model and in Fig. 4 for the cross-sectional top view of the nanowire.

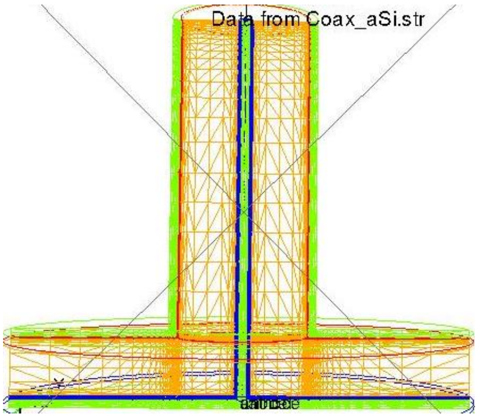

Fig. 3. Coordinate grid of the finite-difference method in the side view cross-section of the solar cell model.

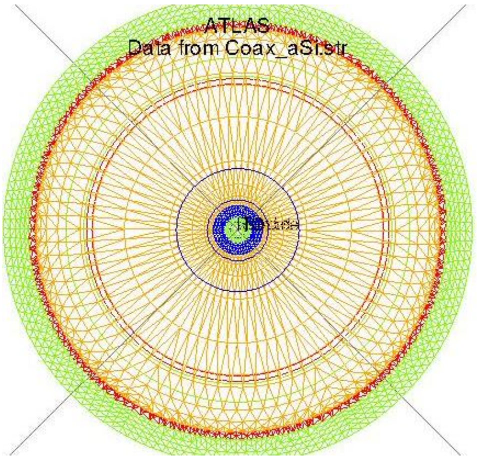

Fig. 4. Coordinate grid of the finite-difference method in the top view cross-section of the nanowire.

An adaptive coordinate grid has increased the density near the *p*-*n* junctions and in other areas where the electric field changed rapidly. The differential equations were discretized using the finite-difference method. In this way, the original continuous model was transformed into a discrete one expressed by coupled systems of algebraic equations. To solve the obtained systems of algebraic equations, a Newton iterative method was used.

3. Numerical results and discussion

The study of the proposed solar cell consists in performing two groups of computer experiments. The first group includes study of the effect of the nanowire height H and the ratio of the radius of the radial section of the basic solar cell R_b to the nanowire radius R_{nw} on the electrical characteristics of the solar cell at normal sunlight incidence. The second group of computer experiments consists in the study of the behavior of the solar cell basic electrical characteristics at oblique sunlight incidence.

The ATLAS component of the Silvaco TCAD software package allows us to calculate current-voltage characteristics of a solar cell based on the drift-diffusion model of charge transfer in semiconductor materials. The most important parameters of a solar cell, such as short-circuit current, open-circuit voltage, fill factor and efficiency, can be determined from the *I*–*V* characteristics.

The *I*–*V* characteristics of the solar cell, reflecting dependence of the cathode current on the anode voltage and obtained for different values of the nanowire height, are shown in Fig. 5 for the case of solar radiation incidence at an angle of 90°. As one can see from this figure, the solar cell current-voltage characteristic depends minimally on the nanowire height at normal sunlight incidence due to the main contribution of the basic solar cell.

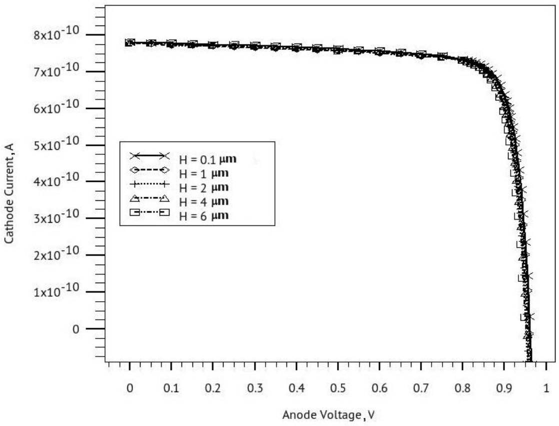

Fig. 5. *I*–*V* characteristics for different nanowire heights at normal illumination.

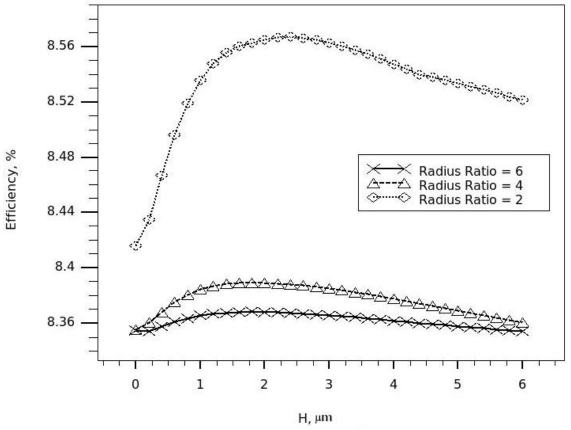

Fig. 6. Dependence of solar cell efficiency on the nanowire height for different ratios of the radii of the basic solar cell and the nanowire.

The dependence of the solar cell efficiency on the nanowire height for different values of the ratio of the radius of the radial section of the basic solar cell R_b to the nanowire radius R_{nw} is shown in Fig. 6 for normal incidence of solar radiation onto the illuminated surface.

It can be seen from this figure that the efficiency slightly increases with the rise in the nanowire height up to a certain maximum value, after which it starts to decrease. This behavior is revealed for all the investigated values of the ratio of the radii of the basic solar cell and the nanowire. The smaller is the ratio of the radii, the higher is the maximum efficiency value. When the radius of the planar *p-i-n* structure of the basic solar cell is twice as large as the radius of the coaxial *p-i-n* nanowire structure, the efficiency reaches a value of 8.57%. In general, increase in the nanowire height has little effect on the solar cell efficiency at normal sunlight incidence. The influence of the nanowire height decreases with an increase in the ratio of the radii of the basic solar cell and the nanowire. Hence, reducing the nanowire density in the array reduces the effect of nanowires at normal incidence of solar radiation.

The study of the influence of the incidence angle of solar radiation on the characteristics of the solar cell is limited by the fact that the three-dimensional model includes only one nanowire and does not allow evaluation of the mutual influence of nanowires in the array. Therefore, when studying the influence of the incidence angle of radiation on the solar cell characteristics, the parameters of the solar cell structure were chosen so to minimize the factors of mutual shading of neighboring nanowires and reflection between them. Therefore, the nanowire height H and the radius of the basic solar element R_b, which indirectly determines the distance between the neighboring nanowires, were set to induce no shading from neighboring nanowires at the sunlight incidence angles varying in the range of 0° to 45° from the normal direction. This condition is satisfied at $H \leq 2(R_b - R_{nw})$.

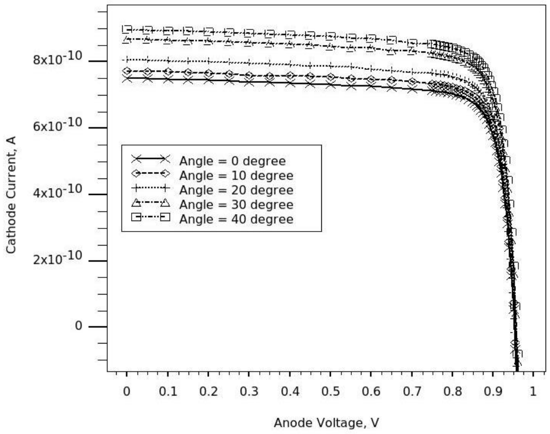

Fig. 7. *I–V* characteristics for different values of the incidence angle of solar radiation.

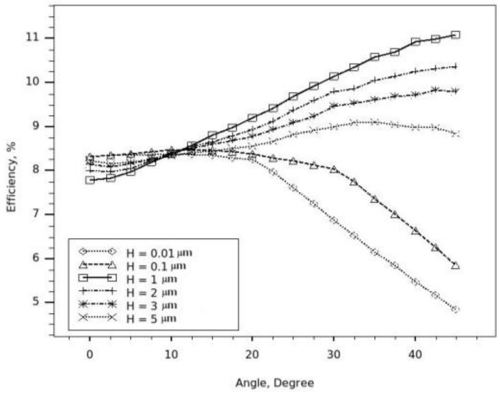

Fig. 8. Dependence of solar cell efficiency on the incidence angle of solar radiation for different nanowire heights.

Fig. 7 shows the current-voltage characteristics of a solar cell with a nanowire height H = 2 μm for different values of the incidence angle of solar radiation. As can be seen from this figure, changing the sunlight incidence angle significantly effects on the current-voltage characteristic, increasing the cathode current when this angle deviates from 90°.

The dependence of the solar cell efficiency on the incidence angle of solar radiation is presented in Fig. 8.

It can be seen from the graphs that at small nanowire heights, the efficiency is the largest at normal sunlight incidence and decreases when the incidence deviates from the normal to the solar cell illuminated surface one. Instead, as the height of the nanowire increases, the solar cell efficiency starts to increase with increasing the angle of deviation of solar radiation incidence direction from the normal one. This effect is most prominent at a nanowire height of 1 μm provided the condition $H = 2(R_b - R_{nw})$ is satisfied. The efficiency increases from 7.8% at normal incidence to 11% at an angle of sunrays inclination of 45°. Such a 30% increase in the efficiency allows us to use this solar cell where normal radiation incidence cannot be ensured, such as on vertical surfaces of buildings, vehicles *etc*.

4. Conclusions

The results of the computer simulations carried out using the Silvaco TCAD software package showed that amorphous Si solar cell structure formed by a vertically oriented nanowire structurally integrated with the basic horizontal thin-film solar cell allows one to enhance the photoconversion efficiency especially at oblique sunlight incidence. This occurs due to the increase of the illuminated surface area and the possibility of independent optimization of nanowire and basic cell structural parameters for normal and oblique illumination. It is demonstrated that at the optimal nanowire height, deviation of sunlight incidence from the normal direction leads to an increase of the solar cell efficiency, such as by 30% at the angle of 45°, due to an increase in the area of the illuminated surface.

The developed solar cell model and the simulation results can be generalized to a solar module consisting of a basic planar thin-film solar cell and a regular array of radial solar cells in the form of vertically oriented nanowires embedded into it. Combining a traditional planar thin-film solar cell and an array of vertical nanowires with coaxial *p-n* junctions in one solar module would allow us to increase versatility of the photoelectric converter due to the mutually orthogonal orientations of the *p-n* junctions and photoactive layers. Such a solar module will be capable to effectively convert solar radiation both at direct and oblique incidence of solar rays. The greatest advantages over traditional solar modules with horizontal *p-n* junctions will be for oblique sunlight incidence due to effective light trapping in a regular nanowires array.

The obtained properties of the solar module allow it to be used for covering horizontal, vertical and inclined surfaces of buildings, transport vehicles, road infrastructure facilities, *etc*., where it is impossible to ensure optimal incidence angle of solar radiation onto the surfaces covered with thin-film solar cells, and solar tracking systems cannot be deployed for technical or economic reasons.

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Authors' contributions

Gnilenko A.B.: conceptualization, methodology, software, formal analysis, investigation, resources, writing – original draft, visualization, writing – review & editing.

Plaksin S.V.: conceptualization, validation, data curation, writing – review & editing, supervision, project administration.

Комп'ютерне моделювання тонкоплівкового сонячного елемента на основі аморфного кремнію з вбудованими нанодротами з коаксіальними переходами

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Анотація. У цій роботі досліджено тонкоплівковий сонячний елемент на основі аморфного кремнію з коаксіальною *p-i-n* структурою у вигляді нанодроту з вертикально орієнтованими *p-n* переходами, вбудованою в структуру плоского базового сонячного елемента з традиційним горизонтальним *p-n* переходом. Із застосуванням програмного забезпечення Silvaco TCAD побудовано тривимірну модель сонячного елемента та отримано його основні електричні характеристики. Показано, що розглянута конструкція сонячного елемента дозволяє значно підвищити ефективність фотоперетворення при похилому падінні сонячних променів.

Ключові слова: сонячний елемент, аморфний кремній, Silvaco TCAD, вольт-амперні характеристики, ефективність сонячного елемента.