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# Simulation of Thin-Film Solar Cells with a CuInSe<sub>2</sub> Chalcopyrite Structure

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Abstract. By using numerical simulation, the operating temperatures of a thin-film solar cell based on CuInSe<sub>2</sub> have been determined and the solar radiation density values, at which stabilization of the temperature operating conditions of the thin-film solar cell is not required, have been optimized. The maximum possible efficiency value of ~14.8 % is achieved under actual operating conditions, and is maintained by the incoming thermal energy as both emitted in this cell and infrared radiation of the sun and the environment. A model of the proposed thin-film solar cell was implemented in the COMSOL Multiphysics program environment with the use of the Heat Transfer Module. The operating temperatures of the solar cell without thermal stabilization under conditions of the diurnal and seasonal variations of both the ambient temperature and the power density of the AM1.5 solar spectrum have been determined. The maximum value of this power density was varied from 1.0 to 500 kW/m<sup>2</sup> when using concentrators. The obtained values of operating temperatures of the thin-film solar cell were used to determine its main parameters in the SCAPS-1D program. The graphs of the operating temperature, efficiency and fill factor of the thin-film solar cell versus the solar radiation density are provided. It is shown that in order to obtain the highest possible efficiency of a solar cell, it is necessary to use concentrated solar radiation with a power density, the maximum value of which should be 8 kW/m<sup>2</sup> in July and 10 kW/m<sup>2</sup> in January. In the case of lower and higher values of power density, an appropriate thermal stabilization of the cell under consideration is necessary. The dependencies of efficiency, fill factor and open-circuit voltage versus the stabilization temperature of the solar cell, temperature gradients at the interfaces of the thermoelectric layer were also calculated. It is shown that by choosing optimal values of the thermal stabilization, the efficiency of the proposed solar cell may be about 15 % or more.

**Keywords:** CuInSe<sub>2</sub> thin-film solar cell, numerical simulation, COMSOL Multiphysics, SCAPS-1D, thermoelectric layer, photoelectric converter, solar concentrator, solar radiation density, current-voltage characteristic, fill factor, efficiency

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# Моделирование тонкопленочных солнечных элементов со структурой халькопирита CuInSe<sub>2</sub>

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Реферат. С помощью численного моделирования определены рабочие температуры тонкопленочного солнечного элемента на основе CuInSe<sub>2</sub> и оптимизированы значения плотности мощности солнечного излучения, при которых не требуется стабилизация температурного

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режима данного элемента. Максимально возможное значение КПД ~14.8 % достигается при реальных условиях эксплуатации и поддерживается за счет поступающей тепловой энергии, как выделяющейся в этом элементе, так и инфракрасных излучений - солнца и окружающей среды. Модель предлагаемого тонкопленочного солнечного элемента была реализована в программной среде COMSOL Multiphysics с использованием модуля «Теплопередача». Определены рабочие температуры солнечного элемента без термостабилизации в условиях сезонного и суточного изменения температуры окружающей среды и плотности мощности солнечного излучения спектра АМ1,5, максимальное значение которой варьировалось в пределах от 1 до 500 кВт/м<sup>2</sup> при использовании концентраторов. Полученные значения рабочих температур тонкопленочного солнечного элемента использовались при определении основных его параметров в программе SCAPS-1D. Приведены графики зависимостей рабочей температуры, коэффициента полезного действия и коэффициента заполнения тонкопленочного солнечного элемента от плотности мощности солнечного излучения. Показано, что для получения максимально возможного КПД солнечного элемента необходимо использовать концентрированное солнечное излучение с максимальным значением плотности мощности 8 кВт/м<sup>2</sup> в июле и 10 кВт/м<sup>2</sup> в январе. В случае более низких и высоких этих величин необходима соответствующая термостабилизация рассматриваемого элемента. Также рассчитаны зависимости КПД, коэффициента заполнения и напряжения холостого хода от температуры стабилизации солнечного элемента, градиенты температур на границах раздела термоэлектрического слоя. Показано, что при выборе оптимальных значений термостабилизации эффективность предлагаемого солнечного элемента может составлять порядка 15 % и более.

Ключевые слова: тонкопленочный солнечный элемент CuInSe<sub>2</sub>, численное моделирование, COMSOL Multiphysics, SCAPS-1D, термоэлектрический слой, фотоэлектрический преобразователь, концентратор солнечного излучения, плотность мощности солнечного излучения, вольт-амперная характеристика, коэффициент заполнения, коэффициент полезного действия

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# Introduction

Special attention in modern solar energy is paid to the search for new semiconductor compounds that could replace single-crystal silicon cells. For example, CuInSe<sub>2</sub> ternary compounds with the chalcopyrite structure can be used as these compounds. Such compounds are being actively investigated as materials for thin-film solar cells. As it is known, light absorption in a solar cell with a CuInSe<sub>2</sub> structure is accompanied by direct optical transitions. Compared to monocrystalline silicon, direct exposure to sunlight is not a prerequisite for efficient operation of a CuInSe<sub>2</sub>-based solar cell. Advantages of CuInSe<sub>2</sub>-based thinfilm solar cells are also homo- and heterojunctions, flexibility, high radiation resistance, environmental safety and cost [1]. The efficiency of such solar cells is approaching 23 % yet [2–4]. However, the used vacuum processes and the emerging technological difficulties in the production of photovoltaic modules with the target efficiency value lead to the fact that the final product cost is increased significantly.

Naturally, one of the crucial tasks is the development of methods for manufacturing low-cost thin-film solar cells (SCs) with acceptable values of efficiency. Development and research in this direction made it possible to create CuInGaSe<sub>2</sub>-based thin-film solar cells with an efficiency of 14–17 % [5]. These solar cells are a finished product for commercialization.

Another crucial task is to increase the efficiency of solar cells and to expand the range of operating temperatures at which these solar cells can be efficiently operated under irradiation with concentrated solar radiation, even in the absence of thermal stabilization. The study of the solar cells parameters when their operating temperature is changed is of a practical interest, since these cells in terrestrial conditions are most often exposed to temperatures ranging from 15 °C to 50 °C and more when using solar radiation concentration systems [6]. Moreover, the performance of a solar cell is affected by temperature, since its operating parameters such as open circuit voltage ( $V_{oc}$ ), short circuit current ( $J_{sc}$ ), fill factor (*FF*) and efficiency are depended on the operating temperature ( $T_{op}$ ) [7].

The purpose of this work is to simulate a  $CuInSe_2$ -based cell under conditions of increased operating temperature by using concentrators and to optimize the values of the solar power density when the maximum possible efficiency of the SCs is maintained in the absence of operating temperature stabilization. To solve this problem, the used software is taken into account whole energy of both released in the cell under study and visible and infrared radiation (IR): the sun and the environment.

# Construction of the thin-film solar cell



The original thin-film solar cell with a CuInSe<sub>2</sub> chalcopyrite structure is shown in the Fig. 1 [8], where the first electrode layer 2, the thermoelectric layer 3 based on CuInSe<sub>2</sub>, the second electrode layer 4, the photoelectric converter 5 and 6 consisting of CuInSe<sub>2</sub> and CdS layers respectively, as well as a transparent electrode 7 are electrically connected and sequentially arranged on the polished face surface of the substrate 1 made of stainless steel. The transparent electrode 7 is comprised of zinc oxide with a band gap of 3.3 eV and a visible light transmittance of more than 80 %.



# Operation algorithm of the thin-film solar cell

The visible part of the input solar radiation transmitted through the electrode 7 is absorbed in the photoelectric converter 5 and 6, which generates electric charges. At the same time, the infrared part of the input radiation heats the photoelectric converter 5 and 6. Moreover, the generated charges in the CuInSe<sub>2</sub> layer of the converter 5 and 6 are separated by the electric field of the p-n junction, which leads to the generation of a photo-electromotive-force (photo-emf) between the transparent electrode 7 and the second electrode layer 4. In addition, the remaining fraction of the photoelectric converter 5 and 6. Therefore, a temperature gradient is generated between the first 2 and the second 4 electrode layers. This gradient induces thermo-electromotive-force (thermo-emf) between the upper and lower sides of the thermoelectric layer 3. That, in its turn, leads to the appearance of the output voltage of the solar cell consisting of photo and thermal EMF between the first electrode layer 2, electrically connected to the underside

of thermoelectric layer 3, and the transparent electrode 7. In its turn, the latter leads to the occurrence of the output voltage of the solar cell consisting of photoand thermo-emf between the first electrode layer 2, electrically connected to the lower side of the thermoelectric layer 3, and the transparent electrode 7.

Since the part of thermal energy in the proposed solar cell is used to increase the efficiency of solar energy conversion, there will be no need to stabilize the solar cell temperature and its efficiency will be as high as possible at the certain value of the power density of the AM1.5 solar spectrum.

# **Computer simulation**

Numerical simulation is usually used for designing of solar cells and batteries based on them using concentrators. Moreover, the maximum possible number of parameters affecting the performance of thin-film solar cells is taken into account. The used COMSOL Multiphysics program environment allows you to take into account all of the specified and/or variable parameters when solving most scientific and engineering problems. The simulation was performed by using the Heat Transfer Module of this program environment [9], in which the developed numerical model of a thin-film solar cell was calculated in the absence of stabilization of its temperature [10, 11]. The calculations were carried out taking into account the diurnal and seasonal variations of both the ambient temperature and the power density of the AM1.5 solar spectrum for the geographical coordinates of Minsk. The values of the solar power density ranged from 1 to 500 kW/m<sup>2</sup> by using concentrators. The average minimum and maximum monthly ambient temperatures data in Minsk (from the site: http://belmeteo.net) were taken into account in the modeling.

The obtained values of the operating temperatures of the proposed solar cell were used in the SCAPS-1D program, the description and calculation procedure of which are given in the literature [12, 13], and the action panel is shown in Fig. 2.



Fig. 2. SCAPS-1D action panel

This program was developed for the numerical solution of the Poisson equation and the continuity equation for charge carriers. It can be used to calculate one-dimensional thin-film solar cells [6, 14]. The physical parameters used in the simulation of each layer of a thin-film solar cell are shown in the Tab. 1.

Table 1

Parameters	Transparent electrode (ZnO)	Layer of photo- electric con- verter (CdS)	Layer of photo- electric con- verter (CuInSe <sub>2</sub> )	Second electrode layer (Mo)	Thermoelectric layer (CuInSe <sub>2</sub> )	First electrode layer (Mo)
Layer thickness d, µm	0.05	0.05	1.00	1.00	1.00	1.00
Bandgap $E_g$ , eV	3.30	2.40	1.04	1.20	1.04	1.20
Electron affinity $X_e$ , eV	4.55	4.45	4.30	4.50	4.30	4.50
Dielectric constant, ɛ	9.00	10.00	10.00	13.60	10.00	13.60
Density of states at con- duction band $N_C$ , cm <sup>-3</sup>	4·10 <sup>18</sup>	$4 \cdot 10^{18}$	$2.2 \cdot 10^{18}$	2.2·10 <sup>18</sup>	2.2·10 <sup>18</sup>	2.2·10 <sup>18</sup>
Density of states at valence band $N_V$ , cm <sup>-3</sup>	4·10 <sup>18</sup>	$4 \cdot 10^{18}$	1.8·10 <sup>19</sup>	1.8·10 <sup>19</sup>	1.8·10 <sup>19</sup>	1.8·10 <sup>19</sup>
Thermal velocity of electrons $v_e$ , cm/s	1·10 <sup>7</sup>	1·10 <sup>7</sup>	1·10 <sup>7</sup>	1.107	1·10 <sup>7</sup>	1·10 <sup>7</sup>
Thermal velocity of holes $v_p$ , cm/s	1·10 <sup>7</sup>	1·10 <sup>7</sup>	1·10 <sup>7</sup>	$1.10^{7}$	1·10 <sup>7</sup>	$1 \cdot 10^{7}$
Electron mobility $\mu_n$ , cm <sup>2</sup> /(V·s)	100	50	100	100	100	100
Hole mobility $\mu_p$ , $cm^2/(V \cdot s)$	25	20	25	50	25	50
Donor concentration $N_D$ , cm <sup>-3</sup>	$1.10^{18}$	$1 \cdot 10^{18}$	$4 \cdot 10^{16}$	0	$4.10^{16}$	0
Acceptor concentra- tion $N_A$ , cm <sup>-3</sup>	0	0	$2 \cdot 10^{16}$	$2.7 \cdot 10^{16}$	$2 \cdot 10^{16}$	$2.7 \cdot 10^{16}$

Physical parameters of the proposed thin-film solar cell

## Analysis of the results

From the graphs shown in Fig. 3, it follows, that with an increase in the solar power density, the maximum value of which varies within 1 kW/m<sup>2</sup> <  $P_{\text{max}}$  < 8 kW/m<sup>2</sup> (in July) and 1 kW/m<sup>2</sup> <  $P_{\text{max}}$  < 10 kW/m<sup>2</sup> (in January), the operating temperature  $T_{op}$  increases even during thermal stabilization (Fig. 3a, curve 1). At the same time, to achieve maximum efficiency of a thin-film solar cell, this cell heating or lighting by concentrated solar radiation is required (Fig. 3b). At the specified simulation conditions, the efficiency has maximum values under the stabilization conditions at  $P_{\text{max}} = 2 \text{ kW/m^2}$  and without it at  $P_{\text{max}} = 8 \text{ kW/m^2}$  (in July) and  $P_{\text{max}} = 10 \text{ kW/m^2}$  (in January). In this case, the fill factor would increase to ~69.6 % (Fig. 3c) and the open circuit voltage would decrease to ~0.49 V (Fig. 3d). With a further increase in the solar power density of  $P_{\text{max}} > 8 \text{ kW/m^2}$  (in July) and  $P_{\text{max}} > 10 \text{ kW/m^2}$  (in January), in order to maintain the maximum efficiency, cooling of the solar cell is required. In the absence of solar cell cooling, the open circuit voltage would decrease and the fill factor

would change slightly. Values of solar power density of  $P_{\text{max}} = 8 \text{ kW/m}^2$  (in July) and  $P_{\text{max}} = 10 \text{ kW/m}^2$  (in January) are optimal when using proposed thin-film solar cell, since in this case there is no need to stabilize its temperature to maintain the maximum value of efficiency.

Similarly, the parameters of the considered solar cell are temperature dependent, with the only difference being that the extremes in the efficiency graphs are more pronounced, i. e., the dependencies of the fill factor have both maxima and minima at  $P_{\text{max}} > 2 \text{ kW/m}^2$  (Fig. 4a, b). However, at sufficiently high concentrations of solar radiation, such as, for example, at  $P_{\text{max}} = 500 \text{ kW/m}^2$  (Fig. 4b, curve 5), the fill factor reaches maximum values already at lower stabilization temperatures (*T*). In this case, the dependencies of the fill factor no longer have a minimum in the considered stabilization temperature range. This efficiency behavior (Fig. 4a) is determined by the opposite direction of the change in the fill factor (Fig. 4b) and by the change in the open circuit voltage (Fig. 4c), which determine the maximum output power of the solar cell together with the short circuit current.



*Fig. 3.* The dependencies of operating temperature (a), efficiency (b), fill factor (c) and open circuit voltage (d) of CuInSe<sub>2</sub>-based thin-film solar cell with the temperature stabilization (curve 1) and without it in the middle of July (curve 2) and January (curve 3) versus the different values of the solar power density

The proposed CuInSe<sub>2</sub>-based solar cell, when exposed to solar radiation with a power density  $P_{\text{max}} = 1 \text{ kW/m}^2$  and stabilization temperatures of more than 50 °C, has an efficiency higher than, for example, the CuInGaSe<sub>2</sub>-based solar cell, proposed in [6], when exposed to solar radiation with the same solar power density (Fig. 4a, curve 1').

According to conducted calculations, the efficiency of the proposed CuInSe<sub>2</sub>based thin-film solar cell with temperature stabilization at T = 77.5 °C reaches 15.02 % when a solar power density is equal to 2 kW/m<sup>2</sup> (Fig. 4a, curve 2). At the indicated power density and the absence of temperature stabilization, the thin-film solar cell heats up to 48.6 °C in July and 29.3 °C in January (Fig. 3a, curves 2, 3). At the same time, its efficiency reaches 14.61 % and 13.43 %, respectively, in July and January (Fig. 3b, curves 2, 3).



Fig. 5 shows the daily changes of the temperature gradients at the upper and lower boundaries of the thermoelectric layer, i. e. between the electrode layers that cause the generation of thermo-emf at  $P_{\text{max}} = 8$  and 10 kW/m<sup>2</sup>, respectively, in July and January. As it can be seen from the dependencies plotted in Fig. 5, the temperature gradient has a maximum value between 13 and 14 hours of the day at the lower boundary of the thermoelectric layer based on CuInSe<sub>2</sub>, and this value in the morning and in the evening is much smaller.

![](_page_6_Figure_4.jpeg)

*Fig.* 5. The temperature gradients of CuInSe<sub>2</sub>-based solar cell at the lower (curve 1) and upper (curve 2) boundaries of the thermoelectric layer without the temperature stabilization in July at  $P_{\text{max}} = 8 \text{ kW/m}^2$  (a) and in January at  $P_{\text{max}} = 10 \text{ kW/m}^2$  (b) during the day

The current-voltage characteristics of the CuInSe<sub>2</sub>-based thin-film solar cell were obtained at average temperatures in July at  $P_{\text{max}} = 8 \text{ kW/m}^2$  (Fig. 6a) and in January at  $P_{\text{max}} = 10 \text{ kW/m}^2$  (Fig. 6b), when stabilization temperature (*T*) is the operating temperature (*T*<sub>op</sub>).

![](_page_7_Figure_2.jpeg)

From the obtained characteristics plotted in Fig. 6c it follows that the cell under consideration at  $P_{\text{max}} = 1 \text{ kW/m}^2$  generates the maximum output power when its temperature is 70 °C, which is the operating temperature in this case (Fig. 3a). A significant increase in the short circuit current up to  $J_{SC} = 435 \text{ mA/cm}^2$  at  $P_{\text{max}} = 10 \text{ kW/m}^2$  (Fig. 6b) compared to  $J_{SC} = (41-44) \text{ mA/cm}^2$  at  $P_{\text{max}} = 1 \text{ kW/m}^2$  (Fig. 6c) leads to a corresponding increase in the output electric power when using a concentrator.

#### CONCLUSION

The performed simulation demonstrates that the proposed thin-film solar cell, when using a concentrator, does not require temperature stabilization at solar power densities, the maximum values of which in July and January are 8 and 10 kW/m<sup>2</sup> respectively. Moreover, its maximum efficiency value is ~14.8 % and its operating temperature during the year varies from ~102 °C to ~106.6 °C. Such an operating temperature is maintained by whole energy, absorbed in this cell, viz. both the infrared radiation of the environment and the visible (sun) radiation, which is not used for photogeneration (which is lost during recombination). Consequently, by choosing a solar concentrator and operating temperatures at any time of the year, it is possible to maintain the optimal operating temperatures.

ture of the CuInSe<sub>2</sub>-based solar cell and to implement a mode with increased output power at a fixed area of this cell. Extreme points on the characteristics of the fill factor, efficiency and other characteristics are caused by the solar cell structure consisting of sequentially connected photo and thermal layers.

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