Simulation of the PEDOT:PSS/Si heterostructure for flexible hybrid solar cells

© A.V. Uvarov[1], A.A. Maksimova[1], E.A. Vyacheslavova[1], A.I. Baranov[1], A.S. Gudovskikh[1,2]

[1] Alferov Saint Petersburg National Research Academic University of the Russian Academy of Sciences, St. Petersburg, Russia
[2] Saint Petersburg State Electrotechnical University „LETI", St. Petersburg, Russia
E-mail: lumenlight@mail.ru

Received May 19, 2023
Revised July 26, 2023
Accepted October, 30, 2023

In this article, photovoltaic parameters of flexible hybrid solar cells (SCs) based on the PEDOT:PSS/Si heterostructure were evaluated. Current-voltage characteristics (I-V curves) of the structure under study were calculated, and optimal thickness of the silicon substrate was determined. The influence of the silicon substrate thickness on the spectral dependence of the external quantum efficiency (EQE) of the PEDOT:PSS/Si SCs structure was studied. It was shown that, when the crystalline silicon substrate thickness exceeds 30 μm, absorption is sufficient for the formation of highly efficient SCs.

Keywords: PEDOT:PSS, Si, solar cells, heterostructures, numerical simulation.

DOI: 10.61011/TPL.2023.12.57583.155A

The key parameters determining the success of developing the solar power technology are high efficiency and low cost of photovoltaic converters. Nowadays, solar cells (SCs) are typically produced by using crystalline silicon wafers because silicon is widely applied in the semiconductor industry and is relatively cheap. Silicon-based solar cells account for more than 90% of the terrestrial photovoltaics market. This is due to easy availability of the material whose reserves in the Earth crust are practically unlimited, high level of the silicon technology development, sufficient resistance of silicon to solar radiation, and the fact that solar cells based on silicon substrates are environmentally safe and do not require special disposal procedures. The highest conversion efficiency was achieved for SCs based on amorphous/crystalline silicon heterostructures. In the last few years, there has been a sharp increase in the number of studies devoted to searching for absolutely new materials that could in the future replace amorphous silicon in constructing heterostructure SCs on crystalline silicon substrates. One of the ways of development may be creating hybrid SCs by using organic electrically conductive material poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS). Among other organic polymer materials, PEDOT:PSS has been most widely studied; the reasons for that were its very high electrical conductivity, transparency, and commercial availability. PEDOT:PSS is potential to replace conductive ITO (indium-tin-oxide) layers, while its semiconducting properties are widely exploited in creating OLED displays. Besides high electrical conductivity, films of this polymer material exhibit high visible-range transparency and high mechanical flexibility. In addition, they may be obtained merely from aqueous solution. PEDOT:PSS has proven itself to be an efficient passivating selective contact on silicon substrates, which potentially enables formation of SCs with promising values of efficiency [1]. To date, the record efficiency of silicon photovoltaic converters based on PEDOT:PSS layers is 16.2%, which is far from 21.30% expected from calculations [2]. In addition, a planar silicon substrate less than 50 μm thick is mechanically flexible and can be used to create flexible SCs [3]. All this indicates that PEDOT:PSS is an attractive material for creating emitters of SCs based on flexible crystalline Si, which is to be a substitute for the *p*-type *a*-Si:H layer [4].

This study was devoted to numerical modeling of the PEDOT:PSS/Si heterostructure in order to optimize the substrate thickness for hybrid SCs based on crystalline silicon. To analytically assess the optical and electrical properties of the PEDOT:PSS/Si heterostructure, numerical simulation was performed using the AFORS-HET 2.5 software designed for modeling semiconductor heterostructures [5]. As the basis, a one-dimensional diode SC model was taken, which comprised the PEDOT:PSS emitter layer and crystalline-Si base. The effect of parasitic series and parallel resistances was ignored in modeling.

By numerical simulation with the AFORS-HET 2.5 code, the band diagram for the PEDOT:PSS/Si heterojunction was calculated. Initial parameters for the PEDOT:PSS layer were taken from experimental data [6,7]. In calculation, optical characteristics of the layers were taken into account, including the light reflection outside and inside the illuminated structure. Minor variations in the grid pitch used in numerical calculations did not significantly affect the results; this confirms sufficient accuracy of the obtained data. The PEDOT:PSS layer refractive index was assumed to be fixed at 1.5; that for silicon was in accordance with its spectral distribution [8,9]. Input calculation parameters are listed in the Table.

Basic simulation parameters of the layers

Parameter	Layer	
	PEDOT:PSS	c-Si (n-type)
Thickness d, μm	0.1	1–1000
Band gap E_g, eV	1.6	1.12
Electron affinity χ, eV	3.5	4.05
Doping level N_d (N_a), cm^{-3}	10^{20}	10^{17}
Lifetime of minor charge carriers τ, μs	–	10

As the substrate material, crystalline silicon with a high doping level and relatively low volumetric lifetime of minor charge carriers (τ) was taken. This was necessary to obtain a higher open-circuit voltage in SC, regardless of the high recombination rate of electron-hole pairs, which makes sense when striving to reduce the silicon substrate thickness.

Band diagram of the PEDOT:PSS/Si structure exhibits discontinuities in the conduction and valence bands, which is typical of heterojunctions of this type (Fig. 1, *a*). This is due to the differences in electron affinities and band gaps of the materials. PEDOT:PSS is known to be a degenerate *p*-type semiconductor whose Fermi level is 80 meV below the valence band top [2]. The space charge region in such a structure is about 100 nm wide and is located mainly in the Si substrate (Fig. 1, *b*).

Based on the obtained band diagrams, the I-V characteristics and external quantum efficiency (EQE) spectra were calculated for different thicknesses of the silicon substrate (Fig. 2, *a*, *b*). In calculating the I-V characteristics, the radiation source was simulated by the solar radiation spectrum with the AM1.5G composition and integral power density of 1000 W/m^2.

The calculations show that both the short-circuit current and open-circuit voltage change significantly with silicon substrate thickness. Based on the EQE spectra, we can see that the SC efficiency in the long-wavelength spectrum part decreases with decreasing substrate thickness. This is caused by that crystalline silicon becomes transparent at small thicknesses, and the major portion of radiation passes through the substrate without participating in generation of electron-hole pairs. However, when SC becomes as thin as 30 μm, its quantum efficiency becomes sufficient in the major part of the solar radiation spectrum. This is confirmed by high values of the short-circuit current and, hence, of resulting efficiency (Fig. 3).

Thereat, the flexibility limit of a planar crystalline silicon substrate (i. e. the conditional thickness at which the curvature radius is 50 mm) is about 50 μm [10]. This evidences that, when the silicon substrate thickness exceeds 30 μm, it is possible to create on the basis of the PEDOT:PSS/Si heterostructure a flexible SC with a high efficiency of solar radiation conversion. Moreover, if the surface is textured, thicknesses of 20 μm may be achieved due to light scattering and enhancement of absorption in the long-wavelength spectrum range [11]. All this opens up opportunities for creating flexible SCs based on crystalline silicon by using the PEDOT:PSS/Si heterostructure.

In the course of this research, we constructed a band diagram of the structure under study taking into account the energy and electrical properties of individual layers. The I-V curves and EQE spectra of hybrid SCs were calculated for different silicon substrate thicknesses. It was shown that, when the crystalline silicon substrate thickness exceeds 30 μm, absorption is sufficient for formation of highly efficient SCs. This promises a possibility of creating SCs based on flexible crystalline silicon substrates by using flexible polymer material PEDOT:PSS as an emitter. The research results may be used in forming flexible hybrid SCs based on the PEDOT:PSS/Si heterostructure, as well as in numerical calculations of similar structures.

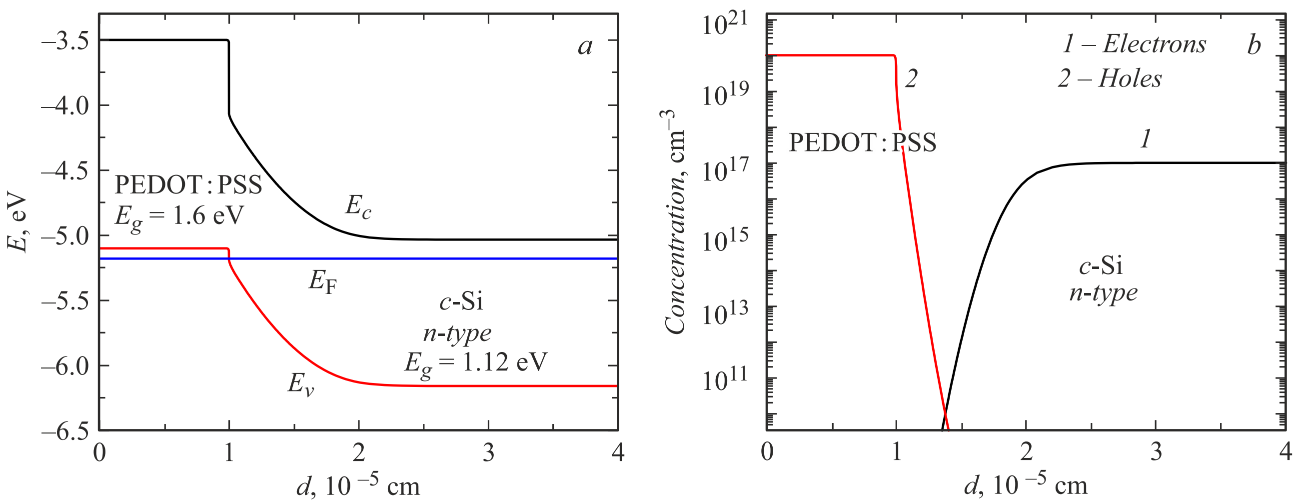

Figure 1. Calculated band diagram (a) and charge-carrier concentration distribution for the PEDOT:PSS/Si heterostructure (b).

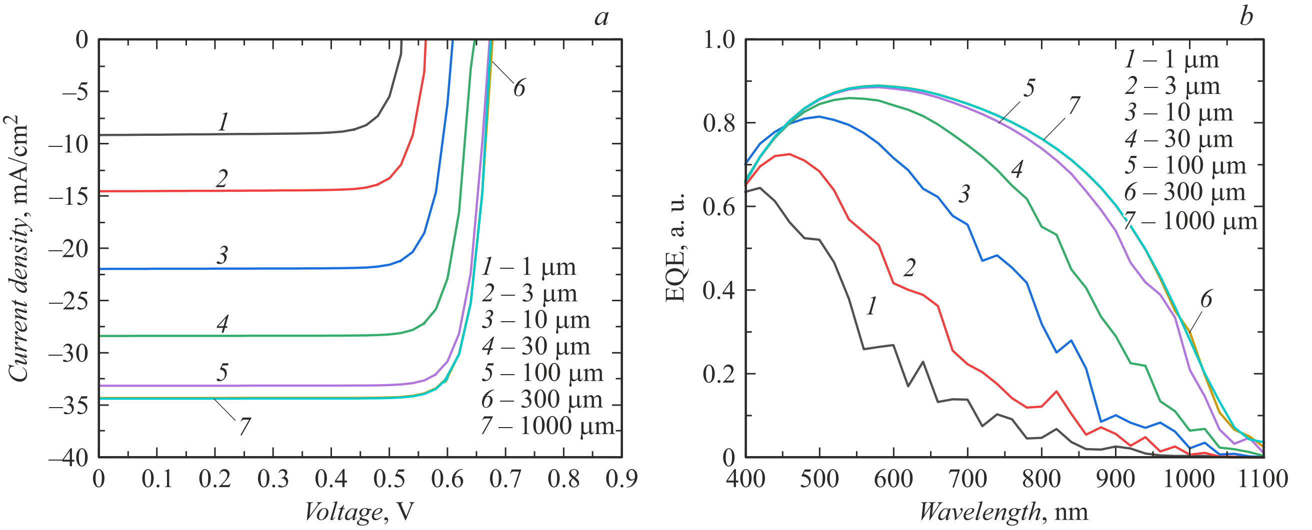

Figure 2. Calculated I-V curves under illumination with the AM1.5G spectrum (*a*) and external quantum efficiency spectra (*b*) for the PEDOT:PSS/Si heterostructures with different silicon substrate thicknesses.

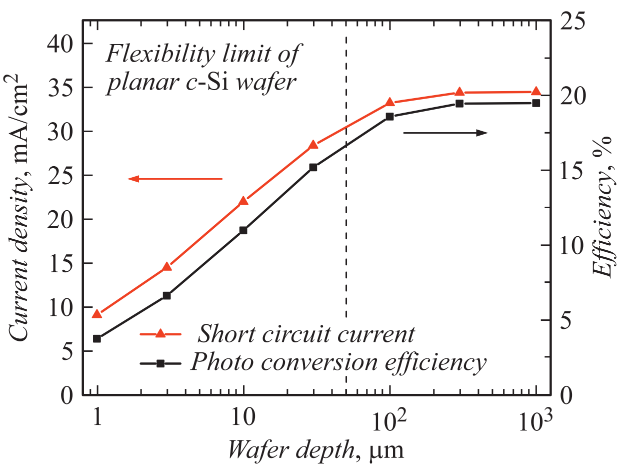

Figure 3. Calculated dependences of short-circuit current and solar cell efficiency on the silicon substrate thickness. The dashed line represents the flexibility limit of the silicon wafer.

Funding

The study was supported by the Russian Scientific Foundation (project № 23-22-00367) (https://rscf.ru/project/23-22-00367/).

Conflict of interests

The authors declare that they have no conflict of interests.

References

[1] A.M. Nardes, M. Kemerink, M.M. de Kok, E. Vinken, K. Maturova, R.A.J. Janssen, Organ. Electron., **9** (5), 727 (2008). DOI: 10.1016/j.orgel.2008.05.006

[2] P. Gao, Z. Yang, J. He, J. Yu, P. Liu, J. Zhu, Z. Ge, J. Ye, Adv. Sci., **5** (3), 1700547 (2017). DOI: 10.1002/advs.201700547

[3] H.-D. Um, I. Hwang, D. Choi, K. Seo, Acc. Mater. Res., **2** (9), 701 (2021). DOI: 10.1021/accountsmr.1c00038

[4] Z. Sun, Y. He, B. Xiong, S. Chen, M. Li, Y. Zhou, Y. Zheng, K. Sun, C. Yang, Angew. Chem., **133** (10), 5092 (2020). DOI: 10.1002/ange.201910629

[5] R. Varache, C. Leendertz, M.E. Gueunier-Farret, J. Haschke, D. Muñoz, L. Korte, Solar Energy Mater. Solar Cells, **141**, 14 (2015). DOI: 10.1016/j.solmat.2015.05.014

[6] L. Groenendaal, F. Jonas, D. Freitag, H. Pielartzik, J.R. Reynolds, Adv. Mater., **12** (7), 481 (2000). DOI: 10.1002/(SICI)1521-4095(200004)12:7<481::AID-ADMA481 >3.0.CO;2-C

[7] S. Jäckle, M. Mattiza, M. Liebhaber, G. Brönstrup, M. Rommel, K. Lips, S. Christiansen, Sci. Rep., **5**, 13008 (2015). DOI: 10.1038/srep13008

[8] C.-W. Chen, S.-Y. Hsiao, C.-Y. Chen, H.-W. Kang, Z.-Y. Huang, H.-W. Lin, J. Mater. Chem. A, **3** (17), 9152 (2015). DOI: 10.1039/C4TA05237D

[9] C. Schinke, P.C. Peest, J. Schmidt, R. Brendel, K. Bothe, M.R. Vogt, I. Kröger, S. Winter, A. Schirmacher, S. Lim, H.T. Nguyen, D. MacDonald, AIP Adv., **5** (6), 067168 (2015). DOI: 10.1063/1.4923379

[10] J.-H. Woo, Y.-C. Kim, S.-H. Kim, J. Jang, H.N. Han, K.J. Choi, I. Kim, J.-Y. Kim, Scripta Mater., **140**, 1 (2017). DOI: 10.1016/j.scriptamat.2017.06.047

[11] Y. Zhang, N. Stokes, B. Jia, S. Fan, M. Gu, Sci. Rep., **4** (1), 4939 (2014). DOI: 10.1038/srep04939

Translated by Ego Translating