Lithuanian Journal of Physics
Vol. **63**, No. 1, pp. 1–7 (2023)

ISSN 1648-8504 eISSN 2424-3647
DOI: https://doi.org/10.3952/physics.2023.63.1.1

MODELLING THE OPTICAL CHARACTERISTICS OF CYLINDRICAL AND ROUGH NANOWIRES WITH SILVER NANOPARTICLES

O. Havryliuk, O. Tkachuk, M. Terebinska, O. Semchuk, and A. Biliuk

Chuiko Institute of Surface Chemistry NAS of Ukraine, 17 General Naumov St., 03164 Kyiv, Ukraine
Email: gavrylyuk.oleksandr@gmail.com

Received 8 July 2022; accepted 18 January 2023

The optical spectra of structures with Ag nanoparticles between rough and cylindrical nanowires are calculated. The simulation was carried out using the finite-difference time-domain method (FDTD). As a source of radiation, a plane wave with the range of wavelengths 300–1000 nm is used. It is shown that with an increase in the root mean square (RMS) roughness of rough nanowires, the absorption coefficient decreases in the range of 500–750 nm due to an increase in the reflection effect. When silver nanoparticles are added, peaks appear at the wavelength of 840 nm (for cylindrical nanowires) and 900 nm (for rough nanowires), which indicates the manifestation of the surface plasmon resonance effect. It is shown that the electric field strength in a system with rough nanowires is higher than in a system with cylindrical nanowires.

Keywords: rough nanowire, cylindrical nanowire, finite-difference time-domain method, optical spectra, metal nanoparticle

1. Introduction

Today, solar energy is a promising area of research. Despite the great achievements, reducing costs and improving the efficiency of solar cells will always be two big challenges in this area. The conversion of sunlight into electricity by photovoltaic technologies is currently a very mature field.

Nanostructured semiconductor devices are promising for use in order to increase the efficiency of energy conversion and reduce the cost of materials. In particular, an effective method for increasing light scattering and trapping in solar cells is based on the use of metallic nanoparticles and nanostructure [1–6].

Silicon nanostructures of different shapes, locations and orientations show interesting characteristics that contribute to their extensive study for use in solar cells [7–11]. Further, nanowires (NWs) have a superior light trapping capability with an efficient charge carrier collection [12, 13]. Structures with silicon nanowires provide a better light absorption compared to that of planar solar cells. The absorption spectrum of sunlight can be controlled by changing the geometrical parameters of the nanowire position [13–15].

An array of metal nanoparticles entails an increase in the wave length of optical light in a solar cell [16–18]. Nanostructures using the plasmon effect improve the optical characteristics of silicon solar cells [19–21]. The size and material of metal nanoparticles can strongly influence the surface plasmon coupling efficiency [17].

The optimal absorption effect is dependent on many parameters, like the material of the particles, the particle shape and size, the array pitch, the shape of the lattice and the distance between the particles and the substrate. All parameters need to be optimized thereby keeping in mind that most parameters are dependent on each other. It is not possible to calculate this analytically, so simulations are needed.

During the synthesis of structures, surface roughness inevitably occurs. Some studies have reported that surface roughness improves light uptake, but other structure parameters may degrade (such as reduced thermal conductivity) [22–24].

The influence of roughness on the characteristics of the structure is significant, so it is necessary to investigate how the roughness affects the optical characteristics of silicon nanostructures. The synthesis of nanowires with a given roughness is described in Ref. [23].

In this article, we will consider the optical properties of structures with rough nanowires and silver nanoparticles. And also let us compare these properties with analogous structures with cylindrical nanowires.

2. Theory

In this paper, we use the numerical method of finite differences in the time domain to solve Maxwell's equations and obtain the optical spectra of the studied structures. The following parameters of Si-NWs and Ag nanoparticles were used for the calculations: the length and diameter of silicon nanowires 2 μm and 100 nm, respectively, and the diameter of silver nanoparticles 100 nm. The correlation length (CL) and the root mean square (RMS) roughness of nanowires are 20 and 5–20 nm, respectively. The surface roughness is generated from a matrix of uniform random numbers in the *k* space. The high frequency components are removed, and the resulting values are transformed back to the real space. A schematic representation of the structures under study is shown in Fig. 1.

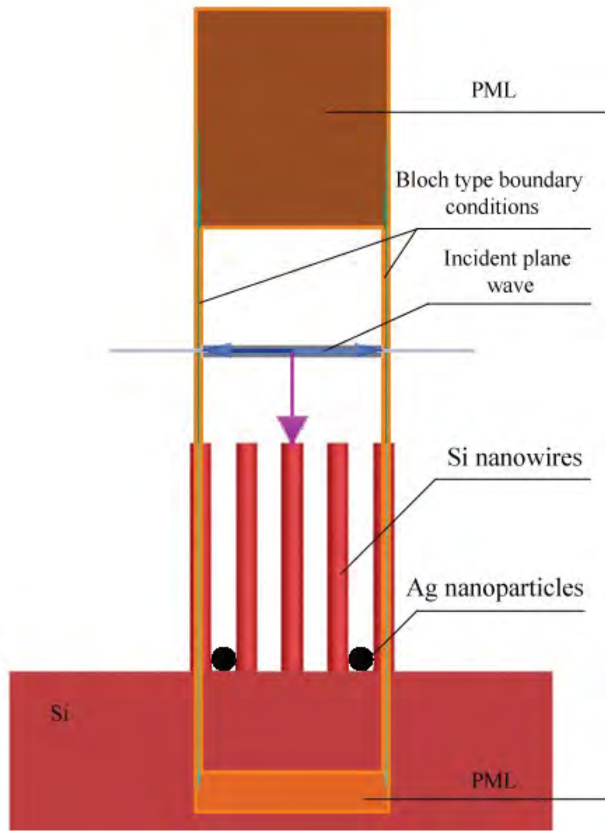

Fig. 1. Cross section of the simulation model.

3. Results and discussion

Let us consider the calculated optical spectra for silicon structures with cylindrical and rough nanowires. The absorption spectra of a structure with silicon nanowires and silver nanoparticles are shown in Figs. 2 and 3. The absorption spectrum without silver nanoparticles is shown in Fig. 2. The absorption spectrum with silver nanoparticles is shown in Fig. 3. Compared with cylindrical nanowires, with an increase in the RMS roughness value in rough nanowires, a significant decrease in the absorption coefficient is observed in the wavelength range of 500–650 nm, as well as an increase of the absorption coefficient in the wavelength range of 400–500 nm (Figs. 2, 3).

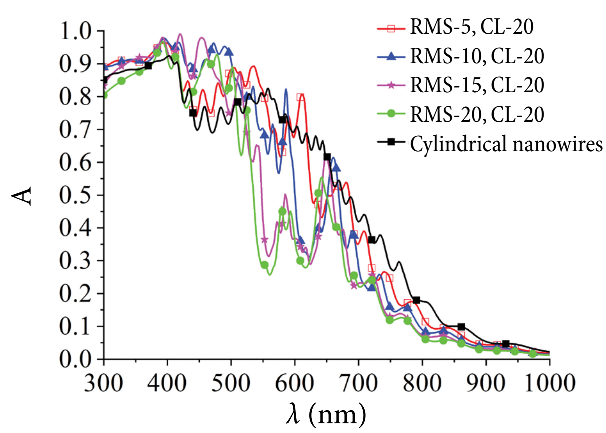

Fig. 2. Absorption spectra of silicon structures with silicon nanowires.

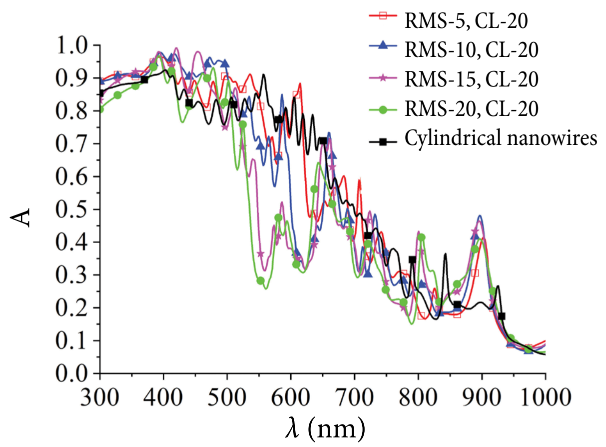

Fig. 3. Absorption spectra of silicon structures with silicon nanowires and silver nanoparticles.

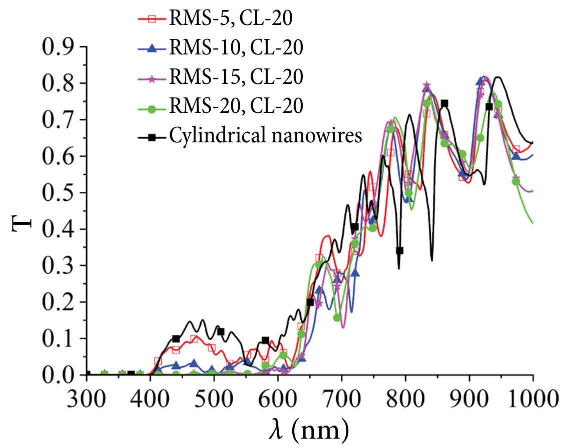

Fig. 5. Transmission spectra of silicon structures with silicon nanowires and silver nanoparticles.

To determine the reasons for such a sharp decrease in the absorption coefficient, the reflection and transmission spectra were calculated (Figs. 4, 5). It is shown that the transmittance in the structures with rough nanowires is lower than in the structures with cylindrical nanowires in the wavelength range 400–800 nm (Fig. 5). An increase in RMS roughness in the structures with rough nanowires leads to an increase in the reflection coefficient in the wavelength range of 500–750 nm. This leads to a significant decrease in the absorption coefficient in the wavelength range of 500–650 nm. Thus, it is necessary to find the optimal parameters of the roughness of nanowires to improve the optical characteristics. Therefore, in our further calculations, we used rough nanowires with RMS roughness = 5 nm and CL = 20 nm.

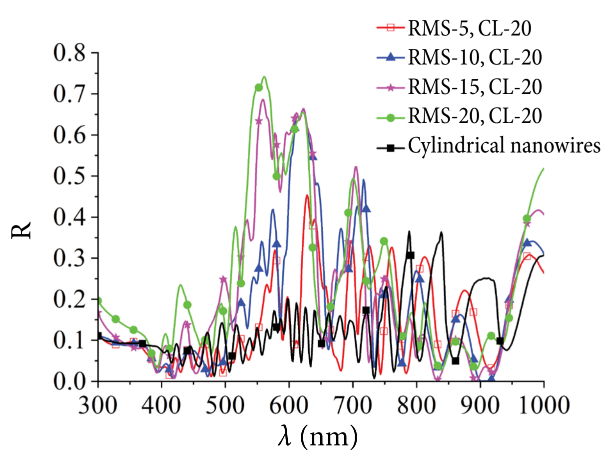

Fig. 4. Reflection spectra of silicon structures with silicon nanowires and silver nanoparticles.

When silver nanoparticles are added to the structure with silicon nanowires, in both cases, additional peaks appear, which may indicate the manifestation of surface plasmon resonance at these wavelengths (Fig. 3). Light scattering at the plasmon resonance frequency is associated with collective oscillations of conduction electrons in the metal [18]. The absorption spectra of only a layer of silver nanoparticles are shown in Fig. 6. These calculations were performed to exclude interference effects that may occur due to the Fabry–Perot effect. It is shown that for a system with cylindrical nanowires it is the appearance of peaks at wavelengths of 840 and 930 nm that is caused by the addition of silver nanoparticles. For a system with rough nanowires, such peaks appear at wavelengths of 820 and 900 nm (Fig. 6). The appearance of additional maxima in the absorption spectra can be interpreted taking into account the possible formation of systems of separated charges of a higher order – quadrupoles and other multipoles. The most intense peaks that may indicate the manifestation of surface plasmon resonance in the system are at the wavelength of 840 nm (for cylindrical nanowires) and 900 nm (for rough nanowires). It can be seen that in a system with rough nanowires and silver nanoparticles the surface plasmon resonance peak is more pronounced and shifted to longer wavelengths compared to a similar peak in a system with cylindrical nanowires (Fig. 6).

In order to verify that light absorption is indeed occurring when the surface plasmon mode is resonantly excited, as opposed to, say,

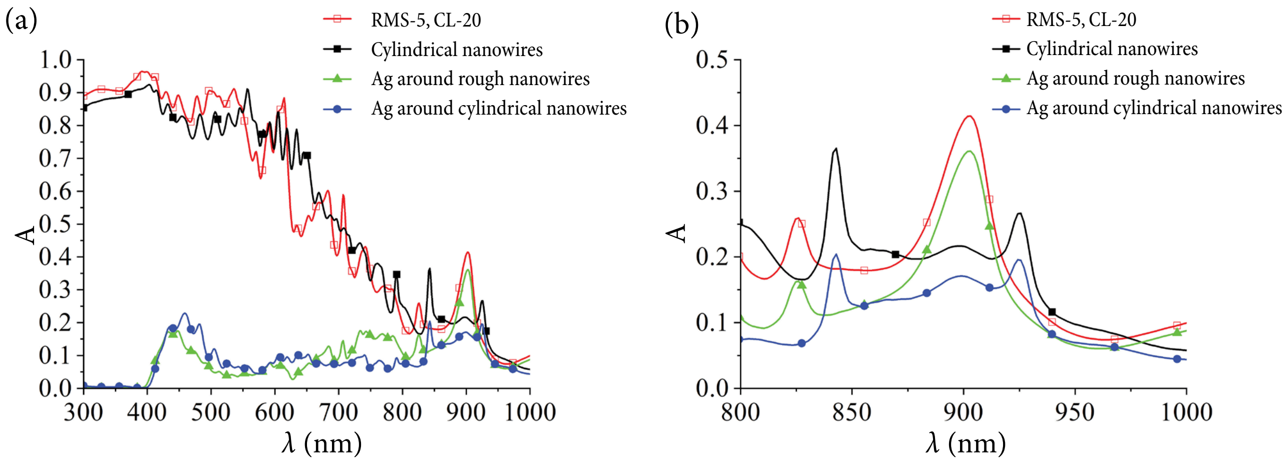

Fig. 6. Absorption spectra of silicon structures with silicon nanowires and silver nanoparticles: (a) the wavelength change is 300–1000 nm and (b) 800–1000 nm.

the excitation of Fabry–Perot resonances or waveguide modes [25], electric field profiles from the simulation results were analyzed. Figures 7 and 8 present the electric field strength distribution at the wavelength corresponding to the surface plasmon resonance of 840 nm (for cylindrical nanowires) (Fig. 7) and 900 nm (for rough nanowires) (Fig. 8).

The presence of metal nanoparticles leads to an increase in the electromagnetic field amplitude in the semiconductor and, consequently, to an increase in the photocurrent response over a wide wavelength range [26].

If the particle is on top of a substrate, the dielectric constant above the particle is different from the dielectric constant below the particle. Fermi's golden rule [27] then says that light is preferentially scattered into a medium with a higher dielectric constant. Two nanoparticles that are closely placed can interact one with another, thereby shifting the resonance of the individual particle [28].

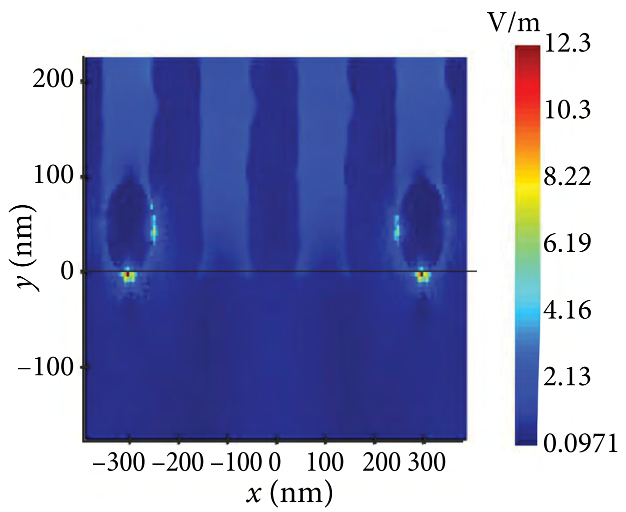

Fig. 8. Electrical field distribution of structures with silicon rough nanowires and silver nanoparticles at the plasmon resonance frequency ($\lambda = 900$ nm).

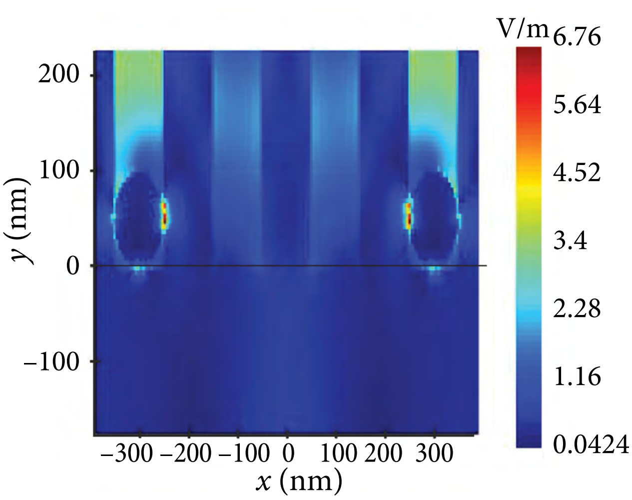

Fig. 7. Electrical field distribution of structures with silicon cylindrical nanowires and silver nanoparticles at the plasmon resonance frequency ($\lambda = 840$ nm).

The type of field distribution in the nanoparticles corresponds to the excitation of electrodipole resonance. The electric field amplification maxima are observed in the area of Si and nanoparticle contact (Figs. 7, 8). Numerical simulation indicates that the electric field strength is significantly higher in a structure with rough nanowires.

For a more detailed analysis, the distribution of the electric field strength along the x coordinate in two different planes was calculated. The first is at the interface between the silver nanoparticle and the silicon substrate and the second is at 50 nm height from the silicon substrate (middle of the silver nanoparticles) (Figs. 9, 10). It is shown that for cylindrical nanowires the intensity of the electric field at the point of contact between the nanoparticle and nanowire is higher than at the point of contact between the nanoparticle and silicon substrate (Fig. 9). But for a system with rough nanowires, on the contrary, the intensity of the electric field at the point of contact between the nanoparticle and nanowire is lower than at the point of contact between the nanoparticle and silicon substrate (Fig. 10).

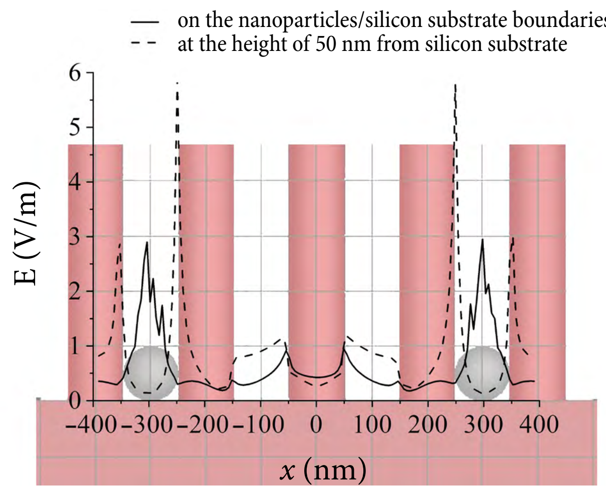

Fig. 9. Electrical field distribution of structures with silicon cylindrical nanowires and silver nanoparticles at the plasmon resonance frequency (λ = 840 nm) by the coordinate *x*.

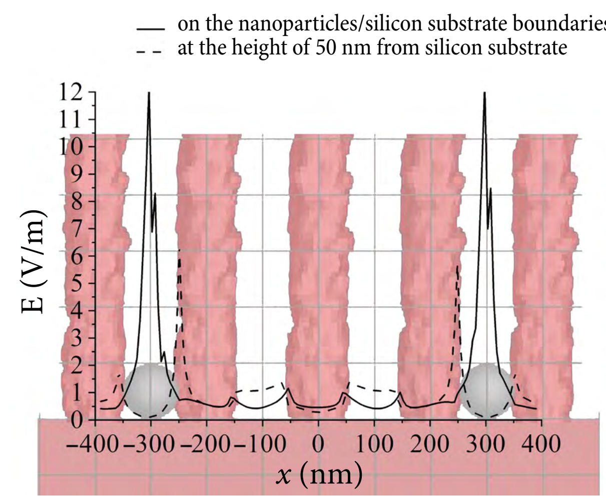

Fig. 10. Electrical field distribution of structures with silicon rough nanowires and silver nanoparticles at the plasmon resonance frequency (λ = 900 nm) by the coordinate *x*.

4. Conclusions

As compared to cylindrical nanowires, with an increase in the RMS roughness value, rough nanowires show a significant decrease in the absorption coefficient in the wavelength range of 500–650 nm, but an increase in the wavelength range of 400–500 nm. For a system with rough nanowires and silver nanoparticles, plasmon resonance peaks appear at wavelengths of 820 and 900 nm. The type of field distribution in the nanoparticles corresponds to the excitation of electrodipole resonance. The electric field amplification maxima are observed in the area of Si and nanoparticle contact. The numerical simulation indicates that the electric field strength is significantly higher in a structure with rough nanowires. The degree of roughness also affects the optical properties, therefore, it is necessary to control the RMS roughness in the manufacture of such structures, because in some cases, the absorption coefficient can significantly decrease due to the strong reflection effect.

References

[1] O.O. Havryliuk, A.A. Evtukh, O.V. Pylypova, O.Yu. Semchuk, I.I. Ivanov, and V.F. Zabolotnyi, Plasmonic enhancement of light to improve the parameters of solar cells, Appl. Nanosci. **10**, 4759–4766 (2020).

[2] F. Enrichi, A. Quandt, and G.C. Righini, Plasmonic enhanced solar cells: Summary of possible strategies and recent results, Renew. Sustain. Energy Rev. **23**(8), 2433–2439 (2018).

[3] R. Ghosh, J. Ghosh, R. Das, L.P.L. Mawlong, K.K. Paul, and P.K. Giri, Multifunctional Ag nanoparticle decorated Si nanowires for sensing, photocatalysis and light emission applications, J. Colloid Interface Sci. **532**, 464–473 (2018).

[4] A. Pal, R. Ghosh, and P.K. Giri, Early stages of growth of Si nanowires by metal assisted chemical etching: A scaling study, Appl. Phys. Lett. **107**, 072104 (2015).

[5] O. Pylypova, O. Havryliuk, S. Antonin, A. Evtukh, V. Skryshevsky, I. Ivanov, and S. Shmahlii, Influence of nanostructure geometry on light trapping in solar cells, Appl. Nanosci. **12**, 769–774 (2021).

[6] R. Zaghouani, S. Aouida, N. Bachtouli, and B. Bessais, Nanoparticles effect on silicon nanowires properties, Chem. J. **1**(2), 10–14 (2015).

[7] F. Es, G. Baytemir, M. Kulakci, and R. Turan, Metal-assisted nano-textured solar cells with SiO_2/Si_3N_4 passivation, Sol. Energy Mater. Sol. Cells **160**, 269–274 (2017).

[8] E. Garnett and P. Yang, Trapping in silicon nanowire solar cells, Nano Lett. **10**, 1082–1087 (2010).

[9] O.O. Havryliuk and O.Yu. Semchuk, Formation of periodic structures on the solid surface under laser irradiation, Ukr. J. Phys. **62**(1), 20–32 (2017).

[10] Z. Huang, S. Zhong, X. Hua, X. Lin, X. Kong, N. Dai, and W. Shen, An effective way to simultaneous realization of excellent optical and electrical performance in largescale Si nano/microstructures, Prog. Photovolt.: Res. Appl. **23**(8), 964–972 (2014).

[11] O.V. Pylypova, A.A. Evtukh, P.V. Parfenyuk, I.M. Korobchuk, O.O. Havryliuk, and O.Yu. Semchuk, Influence of Si nanowires on solar cell properties: effect of the temperature, Appl. Phys. A **124**, 773 (2018).

[12] H. Bao, X. Ruan, and T.S. Fisher, Optical properties of ordered vertical arrays of multi-walled carbon nanotubes from FDTD simulations, Opt. Express **18**(6), 6347–6359 (2010).

[13] R.El. Bashar, M. Hussein, S.F. Hegazy, Y. Badr, M. Farhat, O. Hameed, and S.S.A. Obayya, Analysis of highly efficient quad-crescent-shaped Si nanowires solar cell, Opt. Express **29**, 13641–13656 (2021).

[14] O.V. Pylypova, A.A. Evtukh, P.V. Parfenyuk, I.I. Ivanov, I.M. Korobchuk, O.O. Havryliuk, and O.Yu. Semchuk, Electrical and optical properties of nanowires based solar cell with radial p-n junction, Opto-Electron. Rev. **27**(2), 143–148 (2019).

[15] F. Toor, J.B. Miller, L.M. Davidson, W. Duan, M. Jura, J. Yim, J. Forziati, and M.R. Black, Metal assisted catalyzed etched (MACE) black Si: optics and device physics, Nanoscale **8**, 15448–15466 (2016).

[16] A.P. Amalathas and M. Alkaisi, Nanostructures for light trapping in thin film solar cells, Micromachines **10**(9), 619 (2019).

[17] H.A. Atwar and A. Polman, Plasmonics for improved photovoltaic devices, Nature Mater. **9**, 205–213 (2010).

[18] K.R. Catchpole and A. Polman, Plasmonic solar cells, Opt. Express **16**(26), 21793–21800 (2008).

[19] Y. Li, X. Yan, Y. Wu, X. Zhang and X. Ren, Plasmon-enhanced light absorption in GaAs nanowire array solar cells, Nanoscale Res. Lett. **10**, 436 (2015).

[20] A.A. Biliuk, O.Yu. Semchuk, and O.O. Havryliuk, Width of the surface plasmon resonance line in spherical metal nanoparticles, Semiconduct. Phys. Quantum Electron. Optoelectron. **23**(3), 308–315 (2020).

[21] P.S. Chandrasekhar, H. Elbohy, B. Vaggensmith, A. Dubey, K.M. Reza, V.K. Komarala, and Q. Qiao, Plasmonic silver nanowires for higher efficiency dye-sensitized solar cells, Mater. Today Energy **5**, 237–242 (2017).

[22] L. Cao and K. Sendur, Surface roughness effects on the broadband reflection for refractory metals and polar dielectrics, Materials **12**, 309 (2019).

[23] J.P. Fese, J.S. Sadhu, B.P. Azeredo, K.H. Hsu, J. Ma, J. Kim, M. Seong, N.X. Fang, X. Li, P.M. Ferreira, S. Sinha, and D.G. Gahil, Thermal conductivity of silicon nanowire arrays with controlled roughness, J. Appl. Phys. **112**, 114306 (2012).

[24] Z. Wang, Z. Ni, R. Zhao, M. Chen, K. Bi, and Y. Chen, The effect of surface roughness on lattice thermal conductivity of silicon nanowire, Phys. B Condens. Matter **406**(13), 25152520 (2011).

[25] J.R. Hendrickson, S. Vangala, N. Nader, K. Leedy, J. Guo, and J.W. Cleary, Plasmon resonance and perfect light absorption in subwavelength trench arrays etched in gallium-doped zinc oxide film, Appl. Phys. Lett. **107**, 191906 (2015).

[26] S.H. Lim, W. Mar, P. Matheu, D. Derkacs, and E.T. Yu, Photocurrent spectroscopy of optical absorption enhancement in silicon photodiodes

via scattering from surface plasmon polaritons in gold nanoparticles, J. Appl. Phys. **101**, 104309 (2007).

[27] E. Fermi, Quantum theory of radiation, Rev. Mod. Phys. **4**, 87 (1939).

[28] S. Zou and G. Schatz, Narrow plasmonic/photonic extinction and scattering line shapes for one and two dimensional silver nanoparticle arrays, J. Chem. Phys. **121**, 12606 (2004).

CILINDRINIŲ IR ŠIURKŠČIŲ NANOVIELŲ SU SIDABRO NANODALELĖMIS OPTINIŲ CHARAKTERISTIKŲ MODELIAVIMAS

O. Havryliuk, O. Tkachuk, M. Terebinska, O. Semchuk, A. Biliuk

Ukrainos nacionalinės mokslų akademijos O. O. Čiujko paviršiaus chemijos institutas, Kyjivas, Ukraina