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OPTICAL CHARACTERISTICS OF STRUCTURES WITH SILICON NANOWIRES AND METAL NANOPARTICLES

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To calculate the optical parameters, the finite difference method in the time domain (FDTD) was used, which can be applied to solve Maxwell's equations. A large number of combinations of a planar structure with metal nanoparticles and a structure with nanowires and metal nanoparticles (NPs) were calculated. The height of nanowires *h* varied from 50 to 3000 nm, the period of the structure *P* was 100–600 nm, and the diameter of metal nanoparticles *d* was 50–400 nm. The reduction of light reflection was determined by the anti-reflection effect of the Si-NWs array itself and the direct scattering effect of metal nanoparticles. It was shown that all structures gave significantly lower reflection coefficients compared to that of a solid silicon plate.

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

1. Introduction

Solar energy has advantages in sufficiency and environmental friendliness, therefore it is considered one of the most promising alternatives to traditional energy sources [1].

Thin-film solar cells are used to reduce the cost of photovoltaic production by reducing the amount of active material used. However, due to the low absorption coefficient and insufficient thickness of the active layer, such cells may have a low performance. Therefore, it is important to find ways to improve light capture, which can play an important role in achieving this goal [2].

Periodic lattice structures, photonic crystal structures, nanowires, random scattering surfaces and plasmonic structures are the most widely recognized approaches for light harvesting in thin film solar cells [2].

A silicon (Si) plate reflects one-third of the incident light from its surface, so an anti-reflective coating and various surface texturing methods are used to reduce optical losses [3].

An array of silicon nanowires (Si-NWs) can reduce the reflection loss of incident light and increase the optical path of light, compared to a silicon plate. This makes it possible to achieve an ultra-low reflection coefficient.

The array of Si-NWs is a promising basis for the research of nanostructured solar cells, because by changing the period, length and filling factor, it allows changing the characteristics of the solar cell and creating potentially cheap and highly efficient solar cells.

The solar cell based on Si-NWs has another advantage – the ease of manufacturing a large-area scalable structure. However, the light absorption efficiency of solar cells with Si-NWs is still lower than that of modern Si-based solar cells [1, 4, 5].

Another method of reducing optical losses in solar cells is the use of metal nanostructures on their front surface [6]. This makes it possible to increase the scattering of light into the active medium, which increases the photocurrent of the device [3].

Metal nanoparticles (NPs) strongly interact with visible and infrared photons through the excitation of localized surface plasmons (LSP) [7].

Metal nanostructures attached to the semiconductor photoelectrode cause plasmon resonance, which contributes to the absorption of photons with appropriate wavelengths and transfers excited electrons to the adjacent semiconductor in order to increase the optical response in a wide spectral range [8].

The use of plasmon resonance is an effective method for increasing the efficiency of Si-based solar cells. Metal NPs are promising for improving the efficiency of silicon photovoltaic devices by reducing surface reflection and increasing light trapping in thin-film devices. However, the use of metal NPs can also reduce the efficiency of solar cells, for example, due to the absorption of light inside the NP or due to an increase in the front surface reflectance due to backscattering. Therefore, it is important to properly investigate metal NPs with optimal optical properties for use in silicon photovoltaic devices [1, 7].

The resonance wavelength and intensity of plasmon bands depend on the material of the metal NP, as well as the size and shape of metal nanostructures. By changing the composition, shape and size of plasmonic nanostructures, it is possible to tune the plasmonic bands from the visible to the near-IR region. Thus, it can be concluded that by manipulating the parameters of metal nanostructures, it is possible to tune solar cells in such a way as to increase their efficiency [8–11].

Ag, Au and Cu support LSP excitation when excited by photons with energies below the band gap thresholds of approximately 3.8, 2.4 and 2.1 eV for Ag, Au and Cu, respectively. Conversely, Al supports LSP excitation above and below a narrow range of interband transitions, around 1.5 eV [7].

Cu is one of the important materials in plasmonics. It offers many advantages over other surface plasmon supporting metals. From a plasmonics perspective, it is important to choose a metal that can support a strong surface plasmon at the desired resonant wavelength, especially in the visible region. Cu NPs undergo oxidation and create an interband transition of d-band electrons below 600 nm, but can support surface plasmon resonance in the visible range compared to Ag and Au. Cu NPs are preferred over Au NPs due to their cost-effectiveness, but Cu [10, 12, 13] and Al [3] NPs are difficult to fabricate due to surface oxidation when exposed to the environment [10].

Al NPs have excellent optical properties compared to noble metals and have been reported to be capable of LSP resonance in the UV range and exhibit weak interband transitions near 820 nm, making them a potential candidate for use in far-field light scattering without Fano resonances, compared with NPs of noble metals such as Au and Ag [3, 7].

It has been theoretically investigated that in silicon plates with Al NPs, broadband light trapping occurs, which leads to an increase in photon absorption by 28.7% that is much higher than in Ag or Au [14].

Consequently, Al and Cu have also attracted considerable attention from researchers due to their low cost, widespread presence on our planet, high compatibility and efficient scattering with a tunable plasmon peak.

The purpose of this work is to study the optical characteristics of solar cells based on Si-NWs with Al and Cu NPs, as well as to find the optimal geometric parameters of such structures. The work is useful for further theoretical research and design of a plasmonic thin-film solar cell.

2. Theory

The finite difference time domain (FDTD) method was used to calculate the studied parameters, which can be applied to solve Maxwell's equations. The FDTD method is a powerful numerical algorithm for the direct solution of Maxwell's equations. The advantage of this method is its simplicity and the possibility to obtain results for a wide range of wavelengths in one calculation, as well as the option to set the properties of materials at any point of the calculation grid, which allows considering anisotropic, dispersed and nonlinear media. This method can be accurately applied to general electromagnetic structures, including arbitrarily shaped particles [15–19].

In order to eliminate the non-physical re-reflection of the electromagnetic wave from the boundary of the computational domain and thus model the wave output to infinity in the FDTD method, special absorbing boundary conditions (perfectly matched layer – PML) were used. We applied

Bloch-type boundary conditions to the vertical regions of the computational domain. A plane wave was used as a radiation source. Plane wave sources are used to supply transversely uniform electromagnetic energy from one side of the source region. In our theoretical investigation, we use the solar spectrum AM1.5. The optical parameters of the structure were calculated in a wavelength range of 300–1240 nm.

To find the optimal geometric dimensions of the structure of solar cells, calculations of a large number of combinations of a flat structure with metal NPs and a structure with NWs and metal NPs were carried out. The height of nanowires h varied from 50 to 3000 nm, the period of the structure P was 100–600 nm, and the diameter of metal NPs d was 50–400 nm. The scheme used for theoretical calculations of the structure with Si-NWs and metal NPs is shown in Fig. 1.

3. Results and discussion

After calculating the reflection coefficient for all samples and the average reflection coefficient in the investigated wavelength range, the samples with the lowest reflection coefficient were determined (Figs. 2, 3). It is shown that the structures with a flat surface and Al and Cu NPs have the same geometric parameters. Namely, the diameter of NPs is 150 nm (Fig. 2(a, b)), and the period between NPs is 300 nm (Fig. 2(c, d)).

Similarly, the optimal height of Si-NWs in the samples with NPs was calculated. The result was the same for both types of NPs. The smallest average reflection coefficient was for the structure with the 100 nm height of nanothreads. Calculations were also carried out for NWs with the height in a range of 1000–3000, in which the average reflection coefficient for such high Si-NWs was about 11% for Al NPs and 9–10% for Cu NPs.

The reduction of light reflection is determined by the anti-reflection effect of the Si-NWs array itself and the direct scattering effect of metal NPs. At the same time, the environment has a great influence on the local surface plasmon resonance, so the Si-NWs array affects the resonance wavelength, scattering cross section and direct scattering efficiency of metal NPs. Different particle sizes have different effects on the absorption and reflection characteristics of the Si-NWs array. After introducing metal NPs at the tips of Si-NWs, the scattered light of NPs preferentially combines with Si

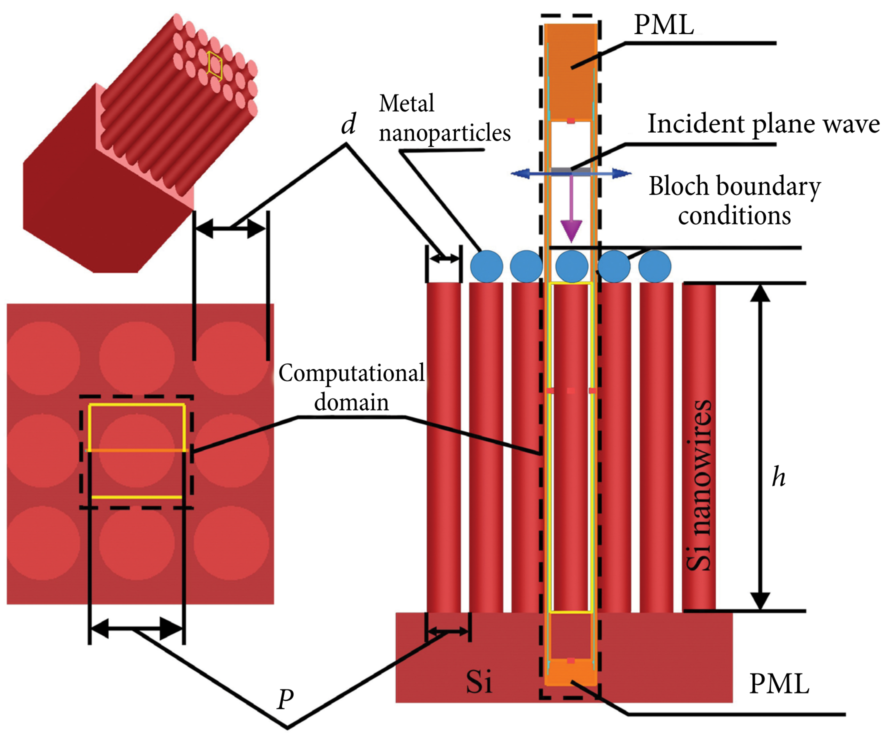

Fig. 1. Cross section of the simulation model with Si-NWs and metal NPs.

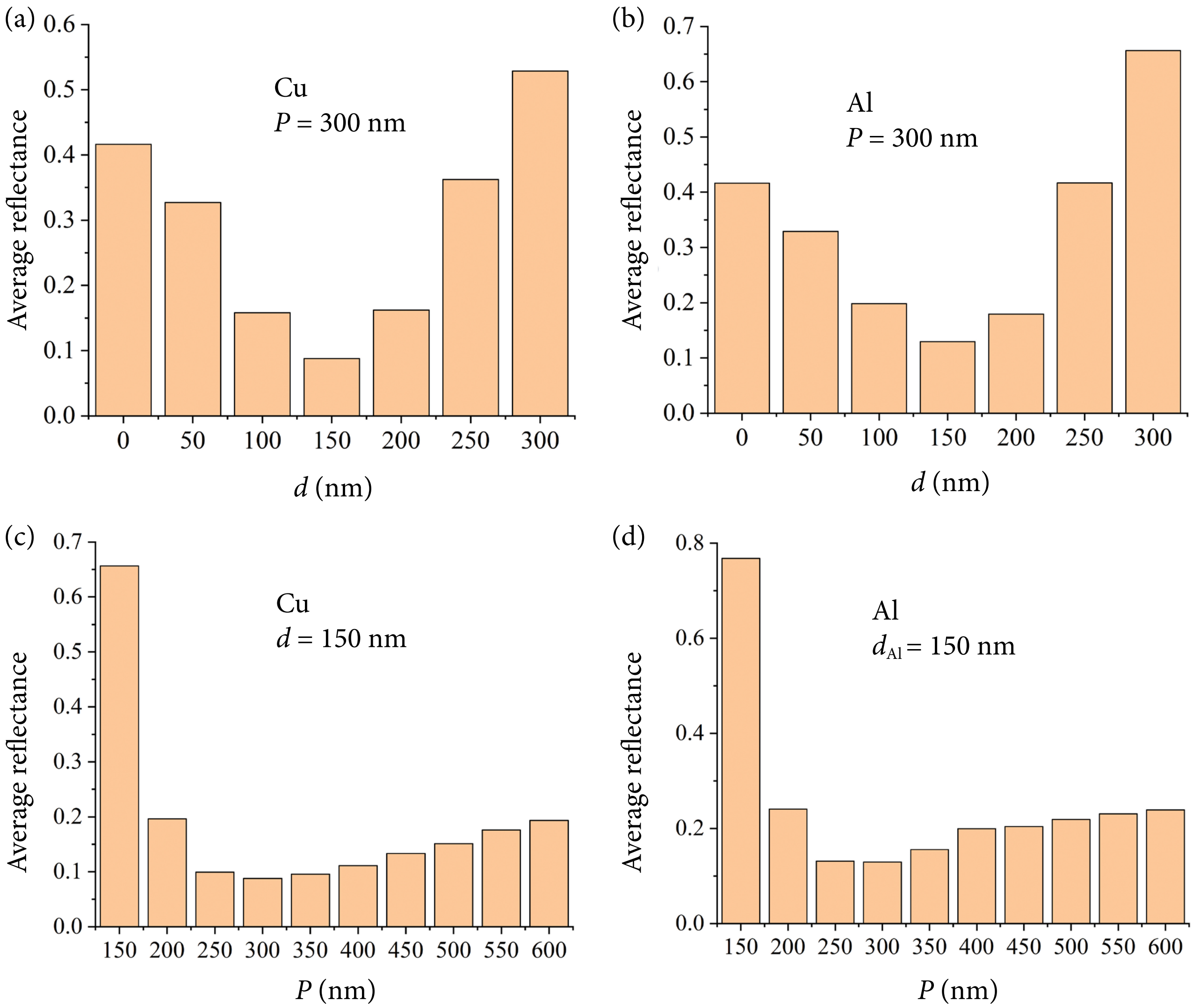

Fig. 2. Average value of the reflection coefficient for various parameters and materials of NPs on the surface of a silicon wafer: (a) change in the diameter of Cu NPs, (b) change in the diameter of Al NPs, (c) change in the period of the location of Cu NPs, (d) change in the period of the location of Al NPs.

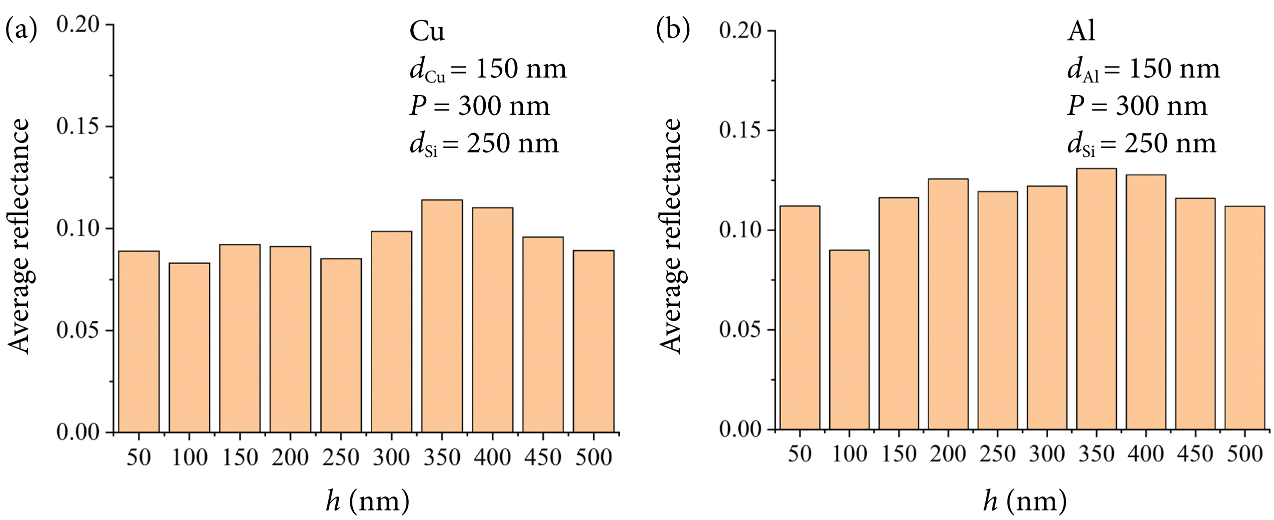

Fig. 3. Average value of the reflection coefficient depending on the height of Si NWs and the materials of NPs on the surface of Si-NWs: (a) Cu NPs + Si-NWs, (b) Al NPs + Si-NWs.

through the near-field coupling between NPs and Si-NWs, so that light absorption is enhanced and light reflection is further reduced [1].

Therefore, based on the set of calculations, the geometric dimensions of the samples with the smallest average reflection coefficient were determined. Namely, the diameter of Al and Cu NPs is 150 nm, the period of arrangement of NPs and NWs is 300 nm, the diameter of NWs is 250 nm, and the height of Si-NWs is 100 nm. Therefore, further studies and comparisons will be conducted for structures with these geometric dimensions.

NPs larger than 100 nm exhibit strong scattering. When they are placed on the surface of the solar cells, the light will be preferentially scattered on the substrate. This increases photon absorption in solar cells in at least two ways. First, preferential scattering reduces light reflection through optical impedance matching, resulting in improved light penetration into the solar cell. Secondly, the light is redistributed inside the solar cells as a result of scattering, which leads to an increase in the length of the light path, which is especially useful for weakly absorbed near-band energy [6].

The reflection, transmission and absorption spectra of the studied structures were calculated (Figs. 4, 5).

Consider the optical spectra of the structure without Si-NWs (Fig. 4). Comparing the reflection spectrum of the structure with Cu NPs and Al NPs, it can be seen that the change in the reflection coefficient for the structure with Cu NPs is small – from 0 to 15% (Fig. 4(a)), but the situation changes for the structure with Al NPs (Fig. 4(b)): the structure

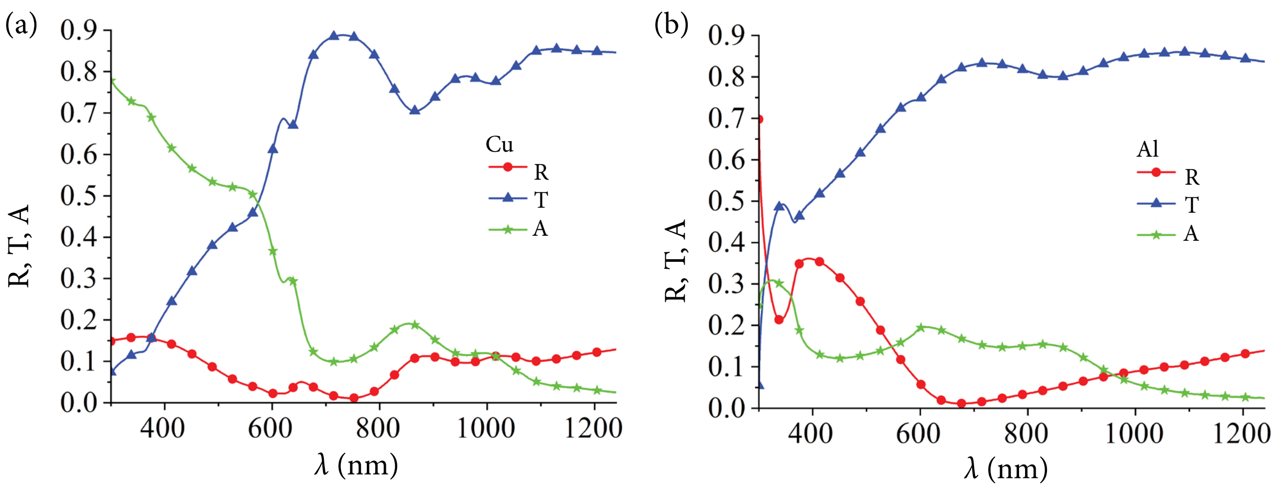

Fig. 4. Reflection, transmission and absorption spectra of the structure of NPs on the surface of a silicon wafer with optimal geometric parameters: (a) Cu NPs, (b) Al NPs.

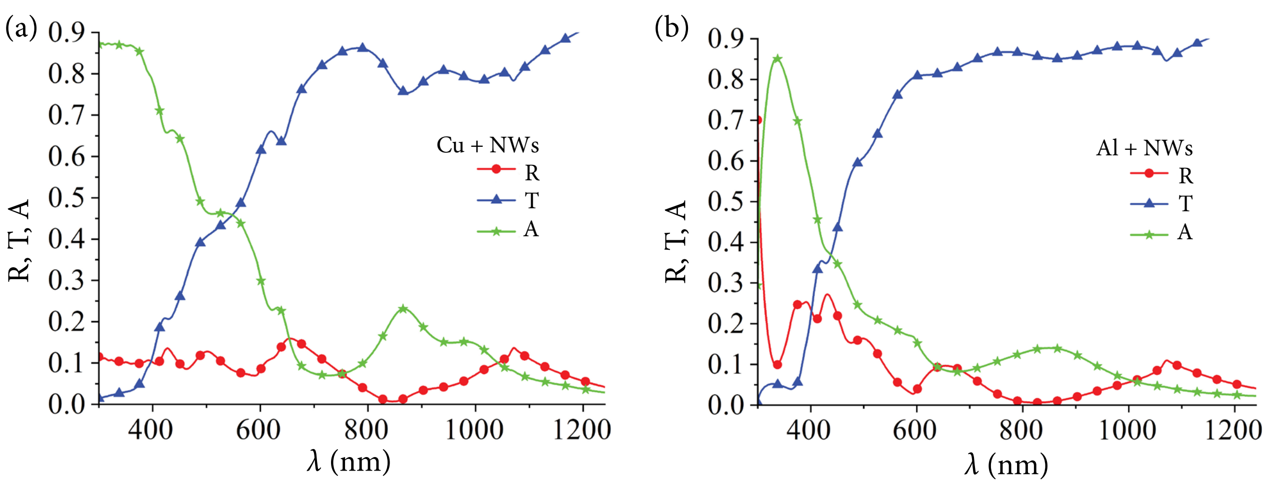

Fig. 5. Reflection, transmission and absorption spectra of the structure of NPs on the surface of Si NWs with optimal geometric parameters: (a) Cu NPs + Si-NWs, (b) Al NPs + Si-NWs.

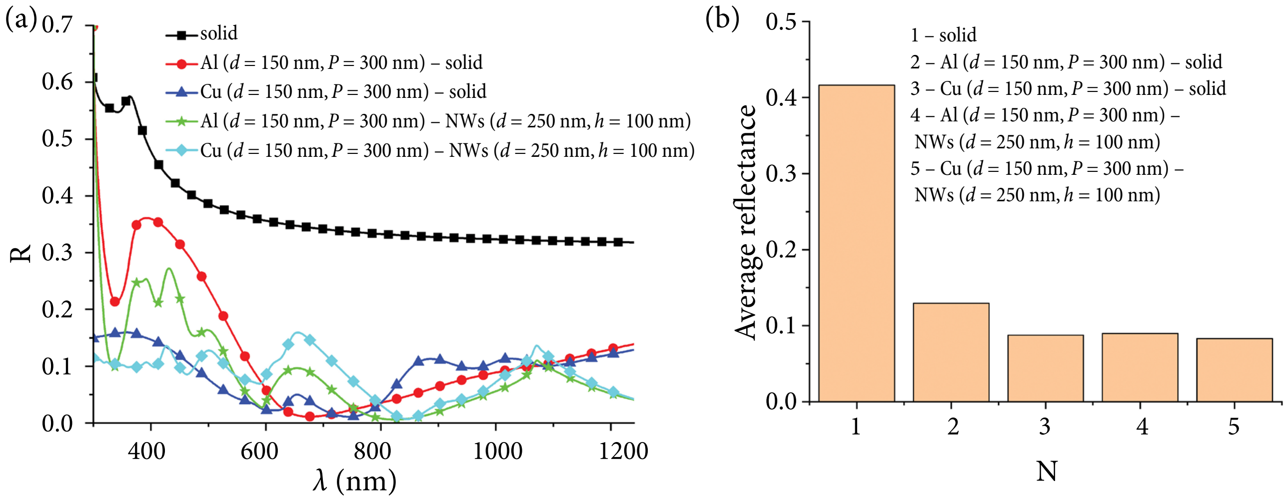

Fig. 6. Comparison of the reflection spectra (a) and the average value of the reflection coefficient (b) for the studied structures.

reflects 70% of light at a wavelength of 300 nm. With a further increase in the wavelength, the reflection coefficient decreases to almost zero at a wavelength of 690 nm and then gradually begins to increase again. That is, in the region of wavelengths up to 800 nm, the structure with copper NPs retains the light better. The absorption coefficient of copper at a wavelength of up to 600 nm is significantly higher than in the structure with aluminum NPs.

The interband transition of Cu occurs at wavelengths less than 500 nm [12]. This strong absorption limits the amount of radiation that reaches the interior of the PV panels and leads to reduced efficiency at short wavelengths for all copper NP-coated PV devices. In this case, the absorption dominates the surface plasmon resonance (SPR), limiting the access of light to the active layer of the device. SPR redshift, broadening, and higher-order multipole excitations are observed in aggregated structures [20]. The SPR red shift can be beneficial because it pushes the plasmonic effect away from the interband transition of Cu. At longer wavelengths when scattering dominates, light is captured by internal reflection.

In the structure with Si-NWs (Fig. 5), the behaviour of the reflection spectrum after 600 nm is similar in both structures, but up to 600 nm we observe a lower reflection coefficient and a better absorption coefficient in the structure with Cu NPs (Fig. 5(a)).

For visual comparison, all reflectance spectra are presented on one graph (Fig. 6(a)). It can be seen that all structures give significantly lower reflection coefficients compared to a solid silicon wafer. It can be seen from this graph that the reflection coefficient is lower in the structures with Cu NPs in the wavelength range up to 600 nm. Figure 6(b) shows a comparison of the average reflection coefficient at all wavelengths. It can be seen that the worst result was in the sample without NWs and NPs, and the sample with Al NPs on a flat surface performed worse. The rest of the samples have almost the same indicators.

The absorption of Si-NWs with metal NPs on the tips of Si-NWs is higher than that of Si-NWs without NPs (Fig. 7), which is due to the near-field coupling between metal NPs and silicon nanomaterials. It is obvious that although different metals have different wavelengths of plasmon resonance, in the absorption spectrum we observe a clear peak of enhanced absorption in the structures with Cu NPs (Figs. 4(a), 5(a), 7), caused by the wavelength of plasmon resonance at a wavelength of 865 nm, and insignificant increase in the absorption coefficient at this wavelength, for the structure with Al NPs (Fig. 7).

For further research, the short-circuit current was calculated for each structure. As can be seen from Table 1, the largest short-circuit current is observed for the structures with copper nanoparticles.

The optical path length of the light can be effectively improved due to the fact that the scattered light acquires an angular distribution in the semiconductor material. In addition, by using a metal reflector as the back contact of the solar cell, light that is weakly absorbed in a single pass can be reflected

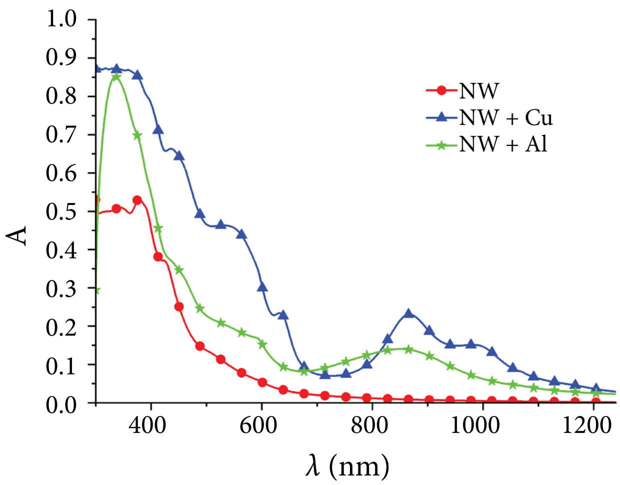

Fig. 7. Absorption spectra of the structure with NWs and metal NPs.

Table 1. Short-circuit current in different structures.

Structure	J_{sc}, mA/cm^2
Si-NWs	7.9
Cu NPs	15.8
Al NPs	12.0
Cu NPs + Si-NWs	14.9
Al NPs + Si-NWs	11.7

to the surface and partially re-emitted by the nanoparticles into the semiconductor layer. Light that is scattered at an angle exceeding the critical angle of reflection remains inside the solar cell. Thus, the optical path length can be effectively increased because the incident light passes through the active layer multiple times, which increases the probability of absorbing scattered light and generating more charge carriers.

4. Conclusions

Based on the set of calculations, the geometric dimensions of the samples with the lowest average reflection coefficient have been determined. Namely, the diameter of Al and Cu NPs is 150 nm, the period of the arrangement of NPs and NWs is 300 nm, the diameter of Si-NWs is 250 nm, and the height of Si-NWs is 100 nm.

Although Cu and Al NPs are difficult to fabricate through surface oxidation, the power conversion efficiency improvements reported by various research groups summarized here suggest that Al and Cu NPs together with Si-NWs may be a promising plasmonic material for our future energy needs.

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DARINIŲ SU SILICIO NANOVIELOMIS IR METALO NANODALELĖMIS OPTINĖS CHARAKTERISTIKOS

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