Modeling of optical characteristics of structures with Cu and Al nanoparticles and Si nanowires

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Introduction

Solar energy has advantages in sufficiency and environmental friendliness, it is considered one of the most promising alternatives to traditional energy sources, in particular fossil fuels. The use of plasmon resonance is an effective method for increasing the efficiency of Si-based solar cells. Metal nanoparticles 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 nanoparticles can also reduce the efficiency of solar cells, for example, due to the absorption of light inside the nanoparticle or due to an increase in the front surface reflectance due to backscattering. Therefore, it is important to properly investigate metal nanoparticles with optimal optical properties for application in silicon photovoltaic devices. Al and Cu have attracted considerable attention from researchers due to their low cost, widespread use on our planet, high compatibility, and efficient scattering with a tunable plasmon peak.

Method

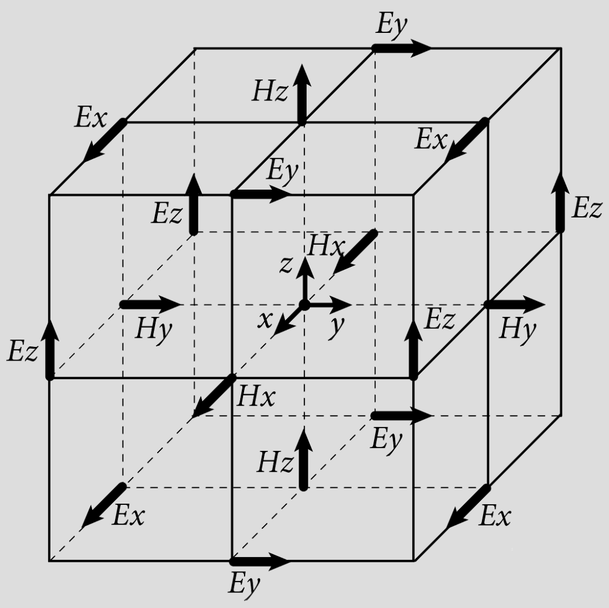


Fig 1. Yee grid pattern.

The finite time domain method (FDTD), which can be used to solve Maxwell's equations and obtain optical spectra of the metal nanostructures, is advantageous due to its simplicity and ability to obtain results for a wide range of wavelengths in one calculation, as well as the ability to set the properties of materials at any point of the calculation grid, which allows to consider anisotropic, dispersed and nonlinear media.

The realization of this method is discrete both in space and in time. The time step is chosen to provide numeric stability and is related to the size of the grid. The presented nanoparticles are described on a discrete mesh consisting of Yee cells (Fig. 1), and the Maxwell equation is solved discretely over time on this grid. For calculations of optical spectra, the following Maxwell equations are used:

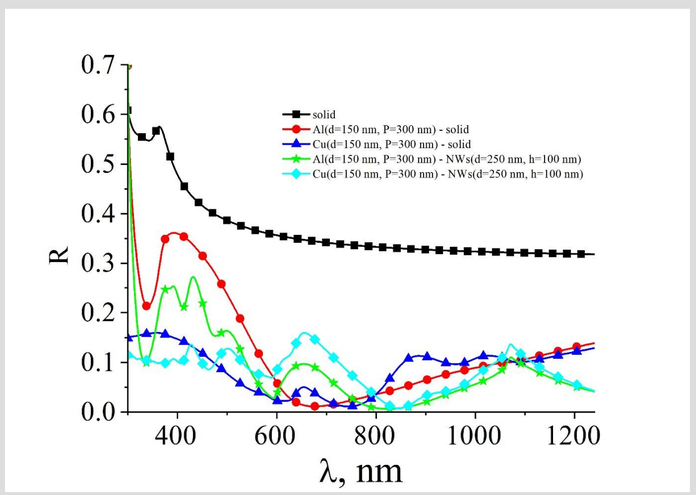
$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon}\left(\nabla \times \vec{H}\right), \qquad \frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu}\left(\nabla \times \vec{E}\right)$$

where *E* and *H* are electric and magnetic fields, respectively, *μ* is the permeability, *ε* is the dielectric permittivity of the medium.

Any change in the field *E* in time is to be associated with a change in the field *H* through space, and vice versa, which is the basis for using the FDTD method. Using the Fourier transform, one can obtain a frequency solution and calculate the transmission, reflection and absorption spectra.

Results

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 nanoparticles and a structure with nanowires and metal nanoparticles were carried out. The height of nanowires (h) varied from 50 to 3000 nm, the period of the structure (P) is 100 – 600 nm, the diameter of metal nanoparticles (d) is 50 – 400 nm.



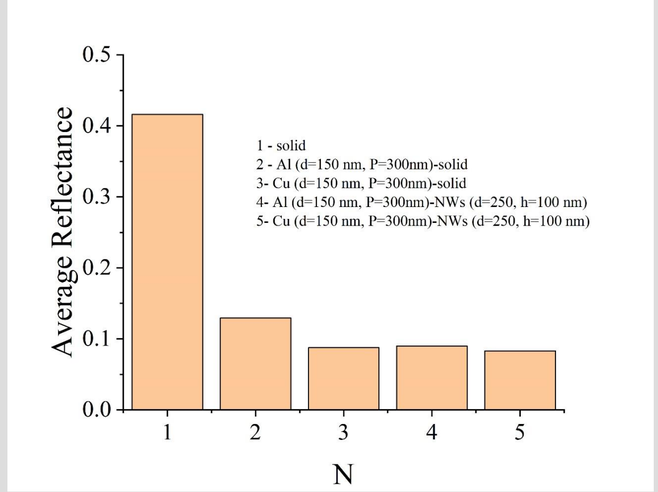


Fig. 2. Comparison of reflection spectra (a) and the average value of the reflection coefficient (b) for the studied structures

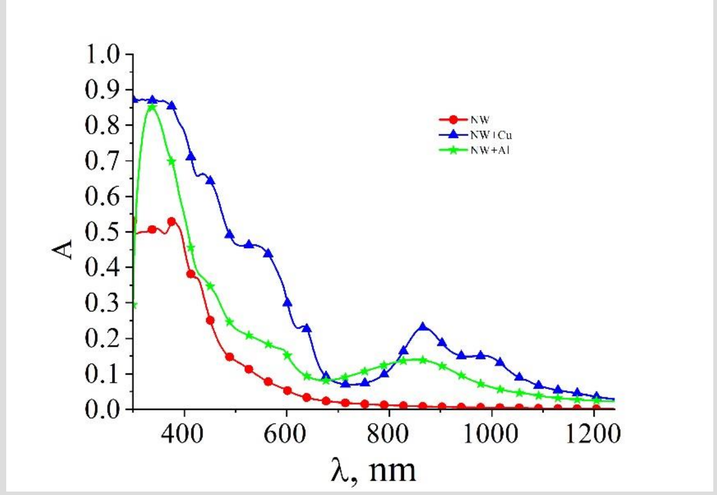


Fig. 3. Absorption spectra of the structure with nanowires and metal nanoparticles

For visual comparison, all reflectance spectra are presented on one graph (Fig. 2a). 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 structures with Cu NPs in the wavelength range up to 600 nm. Figure 2b shows a comparison of the average reflection coefficient at all wavelengths. It can be seen that the worst result was in the sample without nanowires and nanoparticles, 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. 3), 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 structures with Cu NPs, caused by the wavelength of plasmon resonance at a wavelength of 865 nm and not significant increase in the absorption coefficient at this wavelength, for the structure with Al NPs (Fig. 3).