Theoretical modeling of plasmon resonance in structures with metal nanoparticles on the surface

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Introduction

Silicon nanostructures have attracted a great deal of attention and interest because of their potential applications in various fields, such as nanoelectronics, optoelectronics, energy storage, and energy conversion and in biological and chemical sensors.
Many researches have simulated the optical properties of nanowires. But in this work, we first consider some theoretical calculations of localized surface plasmon resonance (LSPR) of silicon nanowires with silver nanoparticles.

Method

There are many methods of numerical electrodynamics. But the most widely used method of electromagnetic modeling is the Finite-Difference Time-Domain method (FDTD). The FDTD method is a powerful numerical algorithm for direct solution of Maxwell's equations. The advantage of this method is the simplicity and the ability to obtain results for a wide range of wavelengths in one calculation, as well as the ability to specify properties of materials at any point of the calculation grid, which allows considering anisotropic, dispersed and nonlinear media. This method can be precisely applied to general electromagnetic structures, including free-form particles. At the same time, the FDTD method can be very resource-consuming, especially when simulating long objects. This method requires 10 to 30 dots per wavelength, while small wavelengths determine a very thick sampling rate. This leads to cumbersome calculations, especially in three dimensions. Therefore, in our calculations, we use two dimensions.
As a source of radiation, a plane wave is used. The sources of plane waves are used to supply transverse-homogeneous electromagnetic energy from one side of the source region. In case of two-dimensional simulation, the source of plane waves is set along the line. In our calculations a range of wavelengths 300 - 1240 nm is used.

Results

As the diameter of the nanowires increases, the transmittance in the shortwave region decreases. There is also a clear decrease in the transmittance at the plasmon resonance frequency. For the nanowire diameter of 100 nm, the peak of the plasmon resonance is at a wavelength of 860 nm. As the nanowires diameter increases, this peak shifts from 840-850 nm (for nanowires with a diameter of 50-80 nm) to 860 nm (for nanowires with a diameter of 100 nm) (fig 1 a, b).
It should be noted that for a structure with 100 nm nanowires and a diameter of 50 nm nanoparticles at the plasmon resonance frequency, the transmittance is at least ~ 20% when for other combinations of the structure it is ~ 40-50% (fig 1).

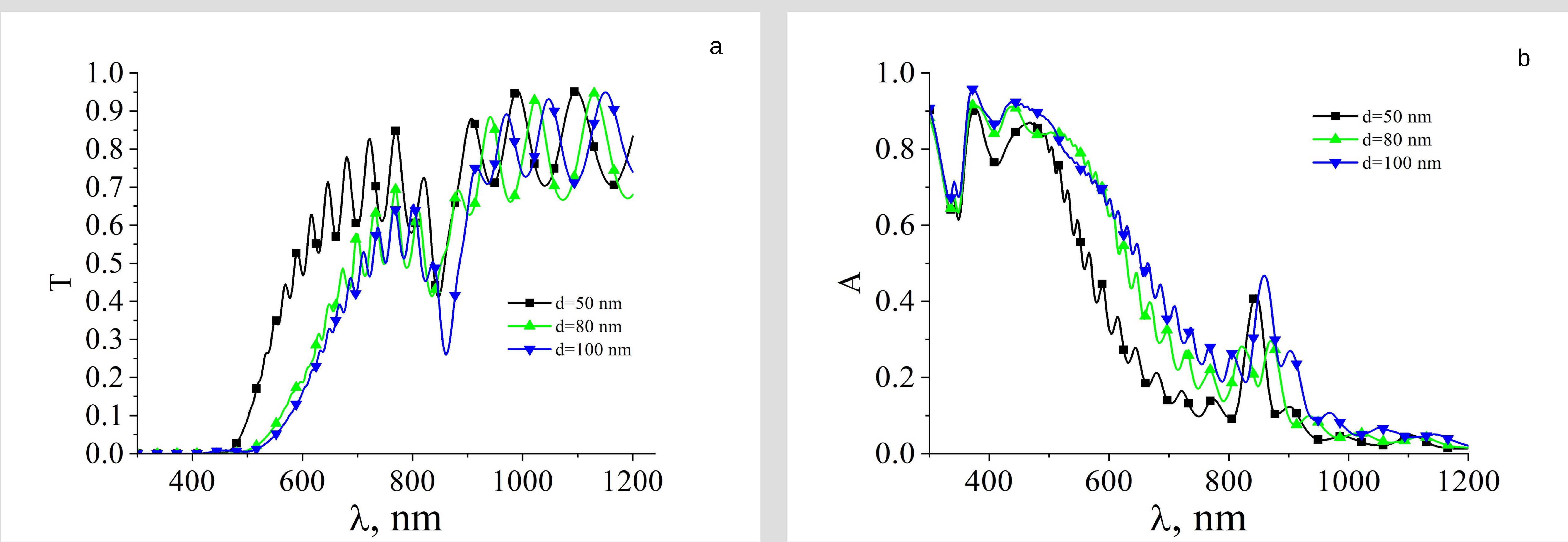

Fig 1. Transmission (a) and absorption (b) spectra of the structure with silver nanoparticles on the surface of silicon nanowires. (d - diameter of nanowires, diameter of nanoparticles is 50 nm, length of nanowires 2300 nm)

In further studies, it is planned to calculate the gain of such structures with and without metal nanoparticles. And also to compare the characteristics of these solar cells with existing analogues.