# FDTD calculation of isolated and arrayed gold nanoparticles optical spectra

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## Introduction

Optical properties of plasmonic nanoparticles, namely gold (Au NPs), is the object of great interest due to plasmon coupling effect, that occurs when two or more particles approach each other. As a result of such interaction the surface plasmon resonance (SPR) band of metal can be shifted to long wavelength region [1]. Upon association (or aggregation) of Au NPs it is possible to shift the absorption in near infrared (NIR) region, that allow the use of infrared light source for activation of photothermal effect of gold in cancer treatment. In this regard the selection of proper morphology of Au NPs and their controlled aggregation remain the challenge, including optimal shape, size and other parameters of nanoarrays.

## Method

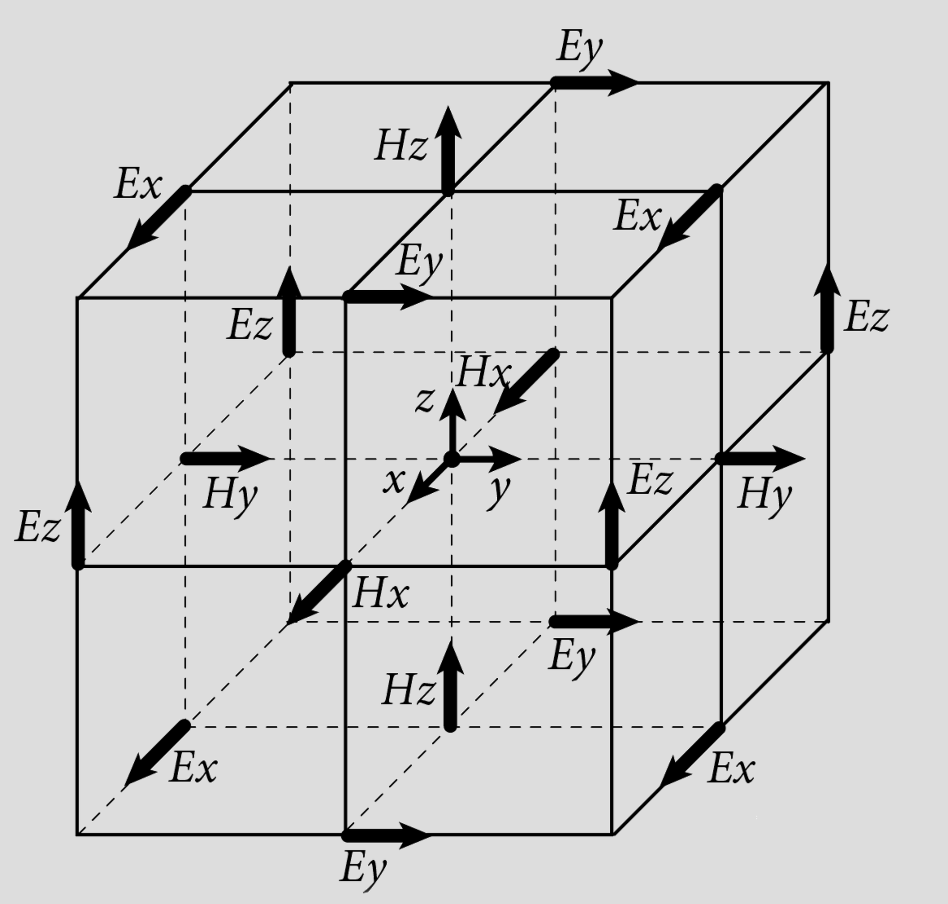


Fig 1. Yee grid pattern.

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, $\mu$ is the permeability, $\varepsilon$ 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

In our study the absorption spectra of isolated Au NPs, as well as an array of Au NPs with different parameters, in aqueous solution were calculated using FDTD method (Fig 2). In particular, for the array of Au NPs with a diameter of 20 nm, with the distance between the particles of 5 nm, the SPR spectra is shown on fig. 3. In this case, the plasmon resonance band maximum appears at a wavelength of 570 nm. By changing the parameters of the system (the nature of the nanoparticles, their sizes and relative spatial location), it is possible to change the positions of the surface plasmon resonance band maximum and predict the optimal parameters of the system for pronounced NIR absorption.

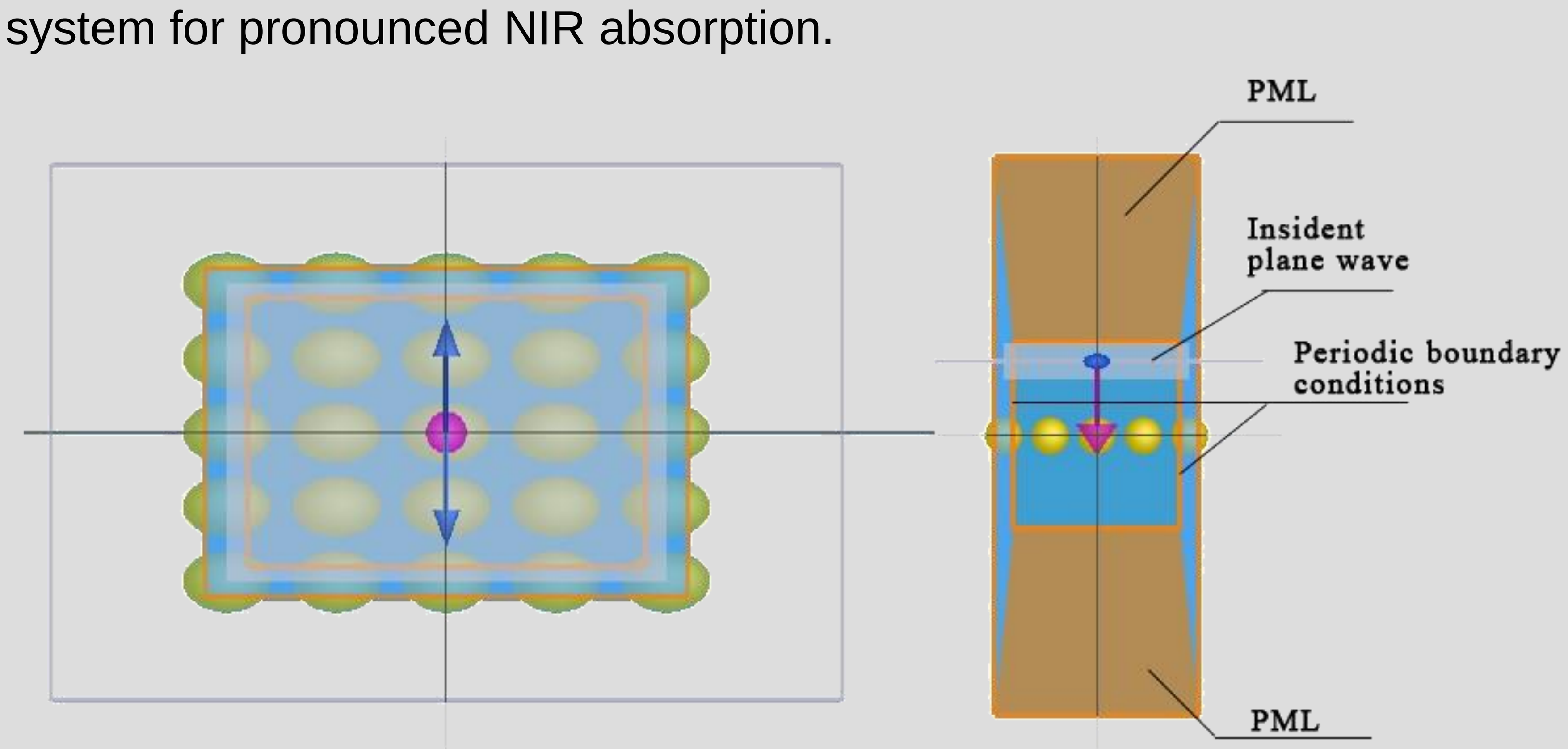


Fig 2. Cross section of the simulation model.

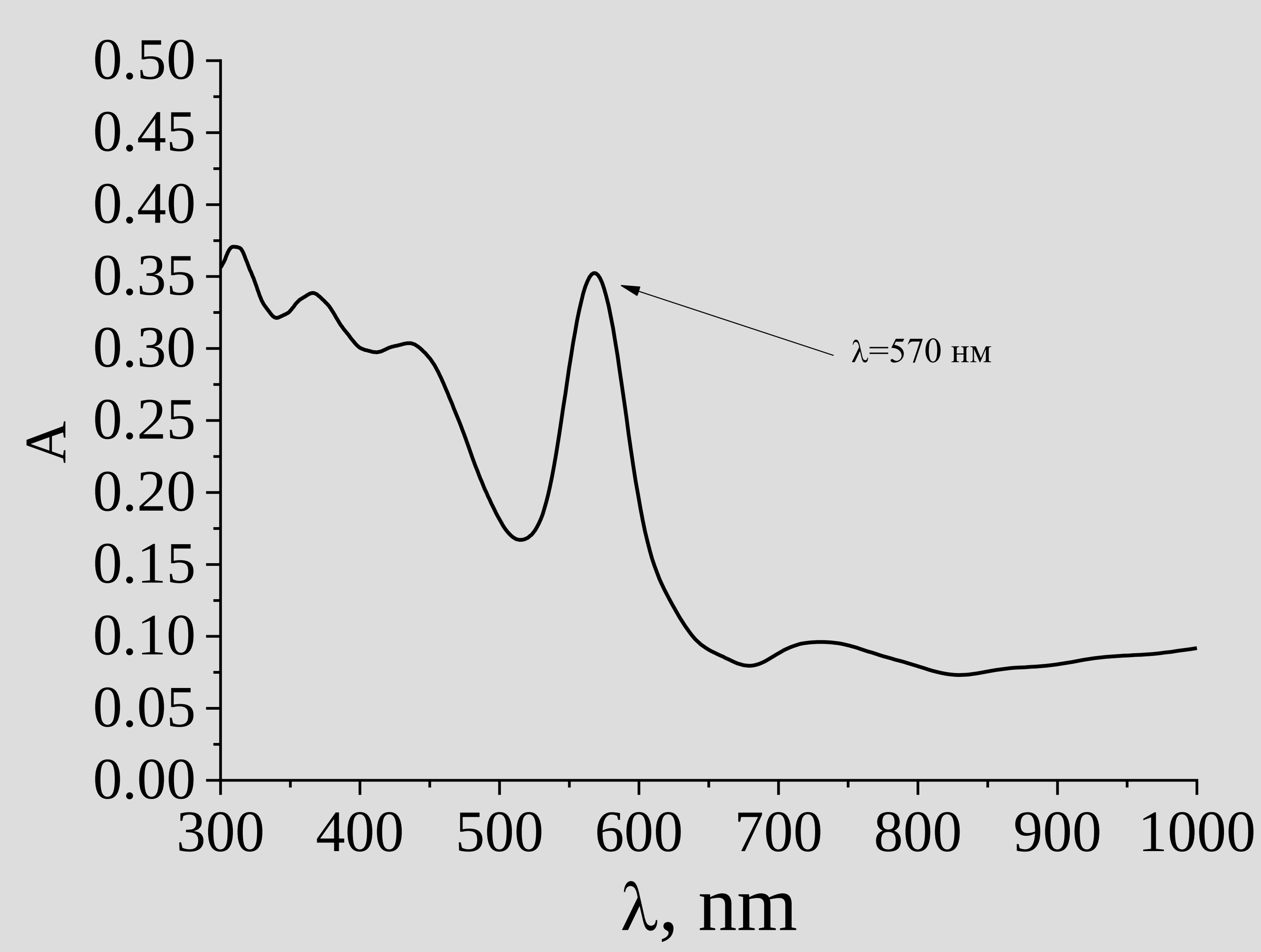


Fig 3. The absorption spectra of an array of gold nanoparticles in aqueous solution

## References

1. Jain, P. K., Huang, W., & El-Sayed, M. A. On the Universal Scaling Behavior of the Distance Decay of Plasmon Coupling in Metal Nanoparticle Pairs: A Plasmon Ruler Equation // Nano Letters.-2007.-**7(7)**.P.2080–2088.