Numerical Analysis on Plasmonic Nano-Cucumber Achieving Large EFs and Wide Tuneability of the Peak

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Introduction:

Researchers in the biomedical field have recently become interested in the potential applications of plasmonics. Surface plasmon resonance based on optical properties of metallic nanostructures can be used for detection of special biological targets. Gold nanostructures with different shapes and sizes have been designed to achieve high enhancement factor (EF), wide range of tuneability of the plasmonic peak, patternabilty and large number of hot spots. The manipulation of these four factors, result in a more efficient platform for biological sensing. The current nanostructures, which includes nanospheres, nanobowties, nanorods and nanostars, have proven to be successful, but they lack large EFs and the wide ranges of tuneability that are required for various applications.

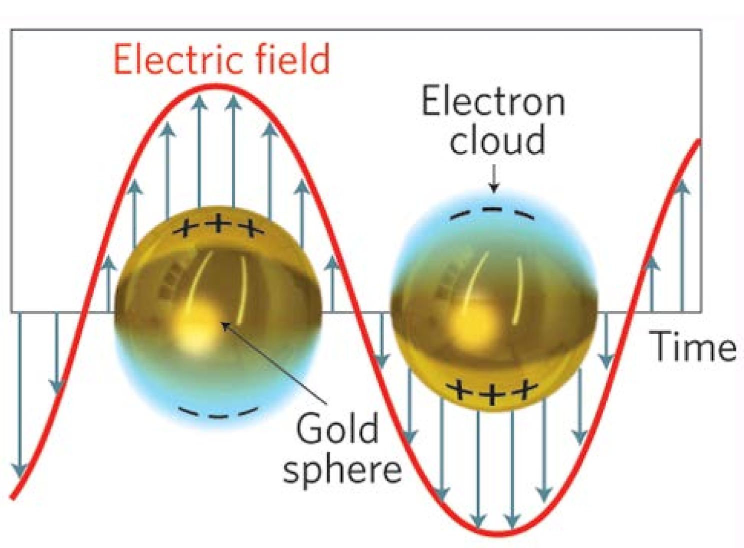

Figure 1. Collective oscillation of electrons with the incident electromagnetic field at a flat gold–air interface[1]

Computational Methods:

In this study, COMSOL Multiphysics is used for the 2D simulation purposes. In the Radio Frequency module, Electromagnetic waves, Frequency Domain is chosen as the physics and Frequency Domain is used as the study. Gold dielectric constant is entered as a function of the wavelength. Geometry is made in the AutoCad software and imported to COMSOL. The Perfectly Matched Layer is used to absorb all outgoing waves. Parametric sweep is also used for computing the problem over a wide range of wavelengths and in the results part, norm of the electric field is considered as the indication of EF and evaluated through the surface maximum in the derived values section.

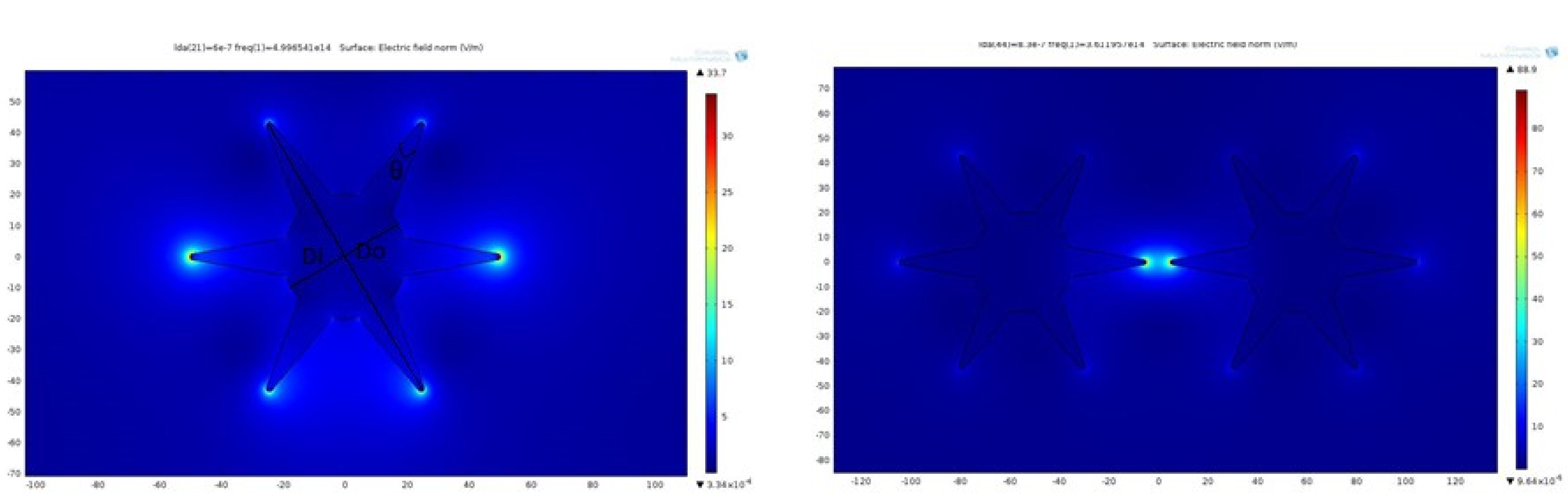

Figure 2. The cross section of single and coupled nanocucumbers. The main factors are introduced.

Results:

For the best design, the research began with comparing different cross sections for single and coupled nanostructures. The coupled design was chosen in order to investigate the coupling effect in the region between two nanostructures. Initially, the cross sections of a circle and polygons, including triangle, pentagon, and hexagon, and nanostars were compared to determine the cross section that produces the highest EF. This simulation resulted in a 6 branched nanostar generating the highest EF and largest number of hot spots.

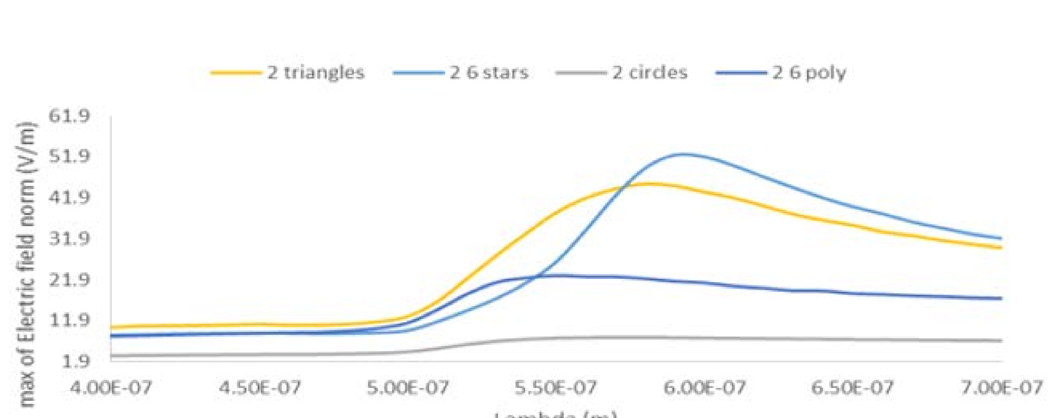

Figure 3. Comparison of electric field produced from 4 different geometric coupled nanoparticles.

The optimization for the nanostar was achieved by considering different values for its size and branch angle. In this regard, main factors were identified to be outer diameter, inner diameter and branch angle which influence the EF and place of plasmonic peak. Then nanocucumber geometry was introduced which allows for the independence of the 3 main factors that could not be achieved in nanostars. An increased EF and red shift for the place of plasmonic peak could be obtained by decreasing the angle, increasing the outer diameter or decreasing the inner diameter.

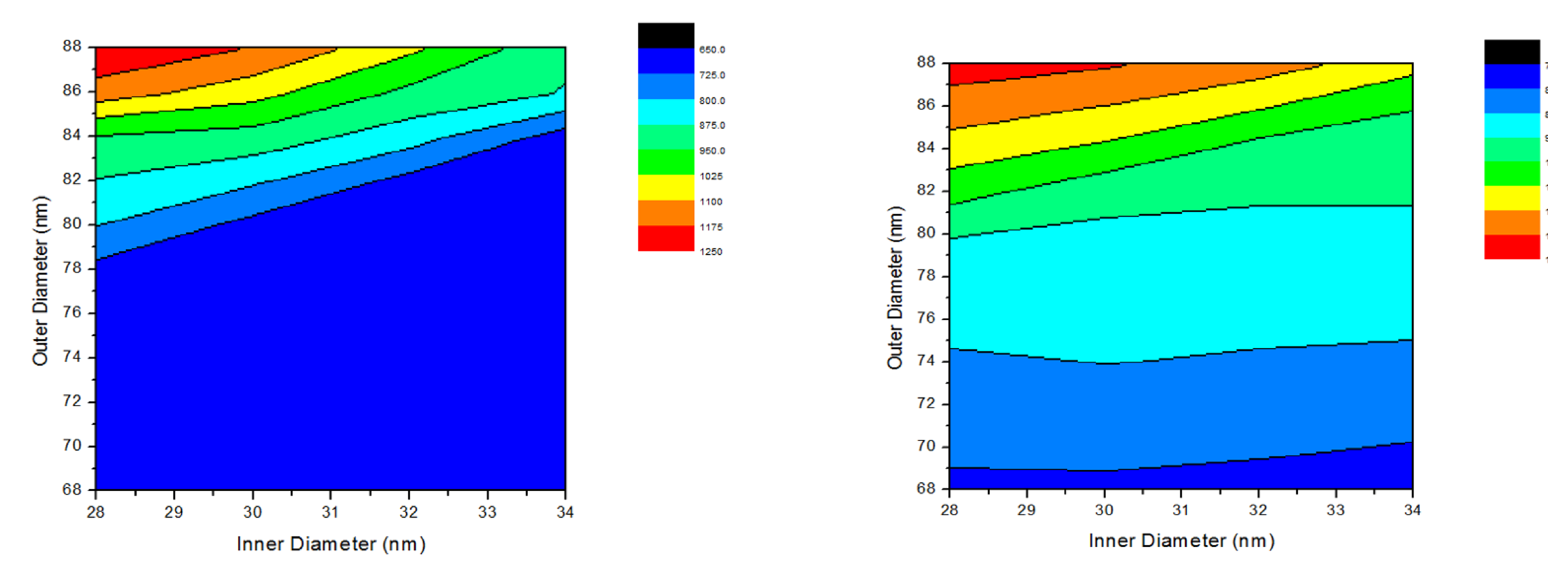

Figure 4. Contour plots of plasmonic peak wavelength in nanometers and Enhancement Factor generated from variations associated with the outer and inner diameter structure of the coupled nanocucumbers.

Among the 3 factors, branch angle had the highest sensitivity for alternating the EF and plasmonic peak wavelength. The inner diameter had little influence over the EF and strong influence over plasmonic peak wavelength which allowed desired control over tuneability. By analyzing a wide range of the 3 factors, the best nanocumcumber candidate was quantified. It produces a large EF while maintaining the plasmonic peak within the range of the biological window.

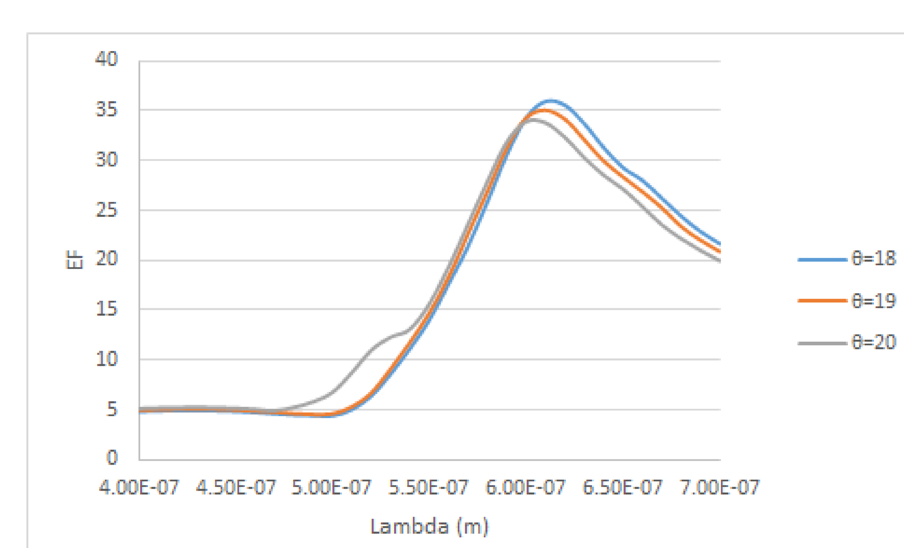

Figure 5. Effect of branch angle on the place of plasmonic peak and EF.

Conclusions:

The unique features of the nanocucumber makes it a strong candidate for the application of ultrasensitive detection of wide range of biological targets. In the future studies, 3D modeling will be simulated and experimental results after the synthesis of gold nanocucumber will be conducted and compared to the simulation results.

References:

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