Journal of Multidisciplinary Engineering Science and Technology (JMEST)
ISSN: 3159-0040
Vol. 3 Issue 1, January - 2016

A Simulation Study of the Plasmonic Resonance of Sharp and Truncated Silver Triangular Nanoprisms

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***Abstract*—Silver nanoparticles have numerous applications in various fields of science and technology. Applications of these materials are highly size- and shape- dependent. In this paper, we have constructed triangular silver nanoprisms using finite-difference time-domain (FDTD) simulation technique to understand the effect of truncation on their plasmonic properties. Along with truncation, effect of thickness and edge lengths were also analyzed for fixed length of snip. Blue shift in dipole plasmon resonance were observed for introduction of truncation, and enhancement in blue shift was observed with increase in snip length. Similarly, for increase in thickness of the prism, a blue shift was observed as well. In contrast to snip length, and thickness studies, increase in edge length has exhibited a red shift.**

Keywords—component; FDTD finit difference time domain; nanoprism;

I. INTRODUCTION

Silver plasmonic nanoparticles have found several applications in various areas of science and technology in the recent years such as sensing and imaging
techniques [1]. Interesting plasmonic properties of anisotropic plasmonic nanoparticles has caused significant interest among researchers towards studying these types of nanoparticles recently of the several shapes of nanoparticles, triangular nanoprisms are of significant interest to us. The interest in triangular nanoprisms mostly arises from the multiple absorption bands in these particles associated with the multiple axes of its triangular shape as each of these axes can support propagating and localized surface plasmon resonance (LSPR) [2], [3]. As a result, Ag nanoprisms exhibit LSPR in different orientations depending on the polarization of the incident light. Further, triangular nanoprisms provide us the opportunity to tune the LSPR properties by suitably modifying their structural parameters such as particle thickness, particle edge length and height [4], [5]. Despite several advantages of triangular nanoprisms mentioned above, synthesis of triangular nanoprisms with absolute precision in edge length, and sharp corners to be employed in desired applications is a challenge. Often times, synthesized triangular nanoprisms do not yield the desired ideal sharp corners; instead they are obtained as structures with one or more truncated corners. Such synthesized truncated triangular Ag nanoprisms were demonstrated as effective biocidal agents [6], [7]]. Also, the truncated triangular forms are more effective than the round or rod shaped nanoparticles with regards to biological interactions. Zheng et al have reported the extinction efficiency of triangular silver nanoprisms in water. They concluded that truncation has introduced blue shift and larger the truncation, higher the blue shift. In that study, they have investigated the plasmon properties of ideal triangular silver nanoprism and truncated silver nanoprisms [8]. For the truncated silver nanoprism, the edge length of 100 nm, thickness 16 nm alone were investigated. Studies regarding the effect of thickness of truncated silver nanoprism, variation of snip length on plasmon properties are scarce to none in the literature to the best of our knowledge Thus we decided to construct triangular silver nanoprism using the finite-difference time-domain (FDTD) simulation technique [9] to gain insights in plasmonic behaviour upon introduction of truncation. Such constructed triangular silver nanoprisms were investigated for various depths of truncation on the dipole plasmon wavelengths. Further we studied the edge lengths effect on plasmonic properties for a fixed truncation.

II. METHOD

A. Finite- Finite-Difference Time Domain Simulations

Conventionally Mie theory was used to solve the Maxwell's equations for small spherical metal nanoparticles in nanometer scale. However, this theory assumes a simple spherical shape for each particle and therefore, does not yield accurate solutions for non spherical nanoparticles and especially with nanoparticles with sharp corners. In order to find solutions for Maxwell's equations for nanoparticles other than spheres, several numerical methods have been developed. Among those numerical methods are Discrete Dipole Approximation (DDA) [10], Multiple Multipole Method (MMP) [11], Modified Long Wavelength Approximation (MLWA) [12], and Finite Difference Time Domain (FDTD) [13] to

name a few. FDTD numerical method is of significant interest for us in our study of the triangular nanoprisms interaction with light. The prime advantage of FDTD is that the user will be able to specify material properties of each of the layers as well as the surrounding medium, the polarization, and frequency of the incident light in the computational domain which results in more realistic solutions. Additionally, this method gives animated displays of electric field movement through the model which gives in depth understanding of interaction of light within the model. Utilizing this numerical method, allows us to model a range of linear and nonlinear materials as well as magnetic materials. FDTD has one inherent advantage over other electromagnetic simulation techniques in that it is performed in time-domain and applies progressive discrete periodical calculations of the electromagnetic field values in time [13]. Said otherwise, FDTD method solves Maxwell's equations for each spatial grid point and at each point of time as the wave propagates through the structure. Time domain approach of the FDTD technique allows the generation of broadband and more accurate output which is useful in producing high quality results with the increase in the complexity of the problem.

The FDTD technique divides time and space into discrete segments. Box-shaped cells are used to segment space. However, wavelength is larger than these spaces. Magnetic fields are located on the faces of the boxes while the electric fields are positions on the edges. This is called the Yee cell field orientation which forms the foundation of the finite-difference time-domain technique [13].

In our study we have taken advantage of the FDTD method. In order to most accurately represent the noble metals of our sandwich structure, Lorentz-Drude dielectric model [14] was used to represent the dielectric function of Ag and Au layers as a function of frequency. For simulation of both the metals six Lorentzian oscillators were used (see equation 1).

$$\varepsilon_r(\omega) = \varepsilon_{r,\infty} + \sum_{m=0}^{6} \frac{G_m \Omega_m^2}{\omega_m^2 - \omega^2 + j\omega\Gamma_m} \quad (1)$$

Where εr,∞ and Ωm are the permittivity at infinite frequency and the plasma frequency, respectively, while Γm, Gm, and ωm are the damping factor (or collision frequency), the oscillator strengths, and the resonant frequency. The reason of choosing Lorentz-Drude model is that noble metals such as gold and silver in our study have multiple plasmonic peaks, which is the best represented by the Lorenz-Drude model. Since, the dielectric of the surrounding medium also has an important effect on the plasmonic properties of any plasmonic structure; we assumed that the surrounding medium is water as plasmonic nanoprisms are often suspended in water as they are used experimentally. The incident radiation in our study was assumed to be a plane wave polarized along the main axis of the nanoprism (i.e. the height of the nanoprism). Further, periodic boundary conditions were assumed in our simulations.

III. RESULTS AND DISCUSSION

Triangular silver nanoprisms constructed using FDTD simulations were investigated for dipole plasmon resonance. Four Ag triangular nanoprisms with snips of 0, 5, 10 and 15 nm were analysed to understand the effect of snipping on dipole plasmon resonance. For Ag triangular nanoprism with snip 0 nm, the dipole plasmon resonance maximum was found at 566 nm. Upon introduction of 5 nm snip, the dipole plasmon resonance maximum had a blue shift to 550 nm. When the snip increased to 10 and 15 nm, the dipole plasmon resonance shifted to 513 and 490 nm respectively. Overall, the trend was, snipping introduced a blue shift in dipole plasmon resonance and larger the snip, farther the blue shift from the triangular nanoprism without snip. The blue shift imparted with snip in triangular nanoprisms can be attributed to decreased length of quantum box for oscillation of electrons [15]. Further it is has been reported in literature that electron density in the corners of a nanoparticle plays decisive role in determining the dipole plasmon resonance wavelength which is often named as the lightening rod effect [16]. Thus, we hypothesize that the observed blue shift may be due to decreased electron density in the corners of the triangular nanoprism as the edges are snipped. No specific trend or pattern was observed for the strength of dipole plasmon resonance peaks with introduction of snipping in nanoprisms. Further, the full width at half maximum of dipole plasmon resonance decreased with increase in snipping for silver nanoprisms.

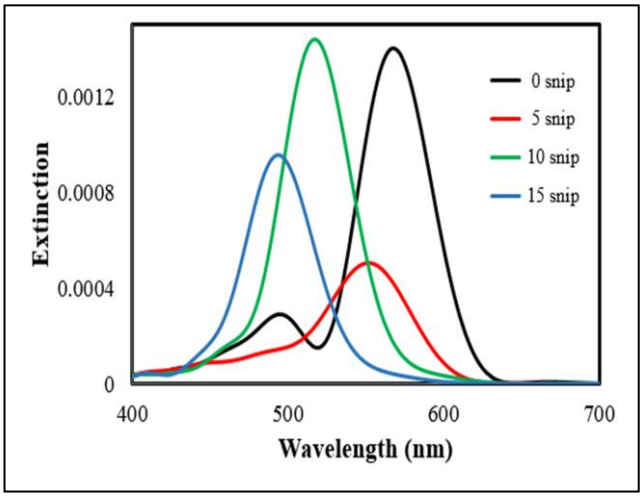

Fig. 1. *FDTD simulation results showing the plasmonic resonance of nanoprism truncated with different snip for prism containing thickness of 30 nm, and edge length 100 nm.*

Followed by analysis of effect of snip on dipole plasmon resonance, we went ahead to understand the effect of edge length on silver nanoprism who thickness and snip kept constant at 10 nm. The edge lengths investigated for this purpose is 60, 80, 100 and 120 nm. When edge length increased from 60 nm to

120 nm a red shift was observed for dipole plasmon resonance for every successive edge length increase of 20 nm. Thus, for edge length of 60, 80, 100, and 120 nm the dipole plasmon resonance maximum was at 494, 523, 548 and 584 nm respectively. The observed red shift for increase in edge lengths are due to lower energy oscillations which are supported by a larger quantum box. The intensity of dipole plasmon resonance peak increased with increase in edge length from 60 nm to 120 nm. This increase in intensity can be attributed to participation of larger number of electrons in oscillations. Beyond the edge length of 150 nm, our simulation studies indicated that the observed red shift becomes less prominent as quantum effects has less significance at such larger edge lengths. Hence, we limited our studies to edge length of 120 nm to take advantage of design tunability. Meanwhile, for the Ag triangular nanoprisms whose edge lengths less than 90 nm, there is severe loss in strength of dipole plasmon resonance peak which limits its applicability to real world experiments.

Followed by investigation of edge length and snip lengths effect on dipole plasmon resonance, we constructed the Ag triangular nanoprism with fixed edge length of 100 nm and snip 10 nm, thickness varied as 5, 10 , 15 and 20 nm.

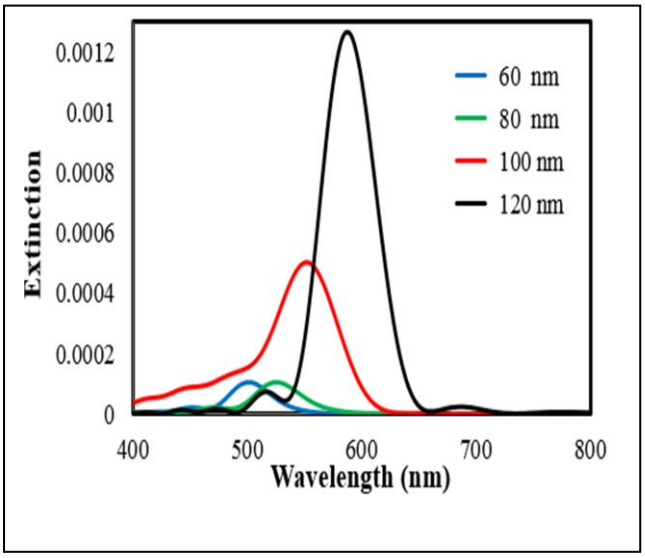

Fig. 2. *FDTD simulation results showing the plasmonic resonance of triangular Ag nanoprism with thickness and snip of 10 nm, for edge lengths 60, 80, 100 and 120 nm.*

Increasing the thickness of nanoprism from 5nm to 20 nm dipole plasmon resonance had blue from 572 nm to 538 nm respectively. Unlike the observations we made with the variation of edge lengths and snips, the intensity of the dipole plasmon resonance was approximately the same for every thickness we analysed.

When thickness of the prism increased, the structure facilitates high energy oscillations in plane perpendicular to edge length. Thus the observed blue shift originated from high energy oscillations (Fig. 3).

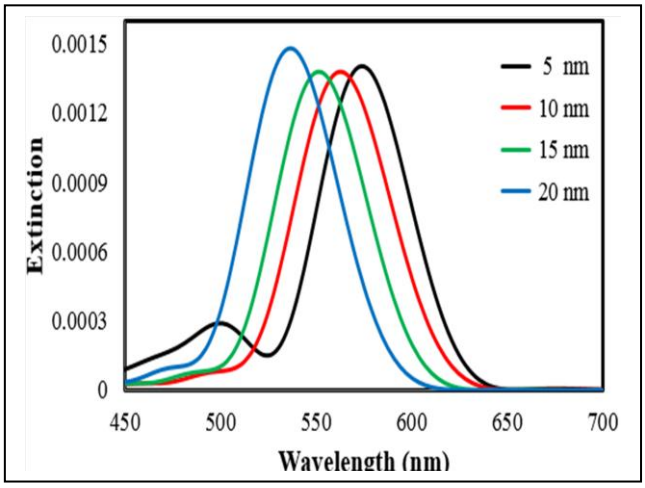

Fig. 3. *FDTD simulation results showing the plasmonic resonance of Ag nanoprism with a fixed edge length of 100 nm, snip 10 nm and thickness ranging from 5-20 nm.*

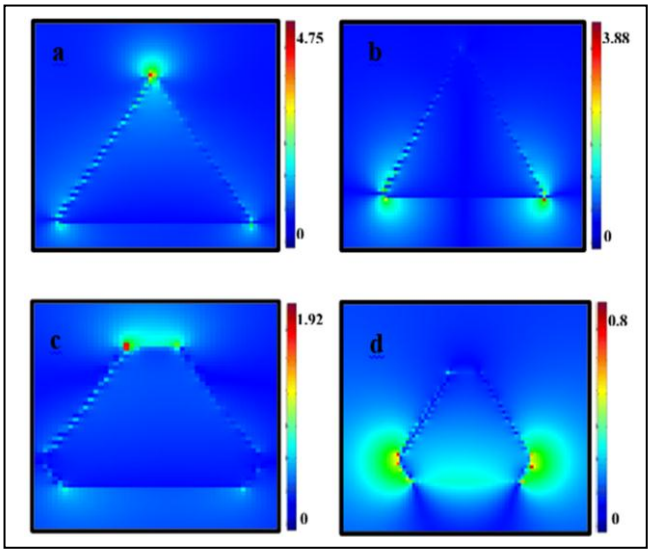

Fig. 4. *The plasmonic enhancement of Ag nanoprism without snipping (a and b) and truncated nanoprism with snip of 10 nm. The edge length (100 nm) and thickness (30nm) were maintained constant in above figure (a – d).*

The plasmonic enhancements for Ag nanoprisms with and without truncation were investigated. In fig 4 (a-b) is ideal triangular Ag nanoprism without truncation, while fig 4 (c-d) a snip of 10 nm was introduced. For fig 4(a-d) the thickness and edge length were 30 nm and 100 nm respectively. In figure 4a and 4c the incident light is perpendicular to the polarization plane, whereas, for fig 4b and 4d the incident light is parallel to the polarization place. The enhancement factor =($|E|^2$in the presence of prism)/($|E|^2$ in the absence) was found to be significantly higher in ideal triangular nanoprism than for the nanoprism with snipping. Further for both triangular nanoprisms with and without snipping, enhancement was very significant

when incident light was perpendicular to the polarization plane than parallel to polarization plane. The enhancement factors calculated for the prisms in figure 4(a-d) are 4.75, 3.88, 1.92 and 0.8 respectively. The reason for higher plasmonic enhancement in triangular silver nanoprism without snipping was due to "lightning rod effect" as the edges are sharper in this case than the truncated nanoprism.

IV. CONCLUSION

This study has determined the effect of truncation on the plasmonic resonance of Ag triangular nanoprisms. Using the finite-difference time-domain (FDTD) simulation technique, perfect Ag triangular prisms and Ag truncated triangular prisms were designed and simulated to understand the role of truncation on plasmonic properties. Introduction of snipping in silver triangular nanoprism has introduced a blue shift and increasing the depth of truncation has increased the blue shift further. No trends in strength of dipole plasmon resonance peaks were observed. Similar to truncation, increment in thickness from 5nm to 20 nm has caused a blue shift. In contrast to effect of truncation, the intensity of dipole plasmon resonance for all thicknesses was constant. to compare the . When edge lengths were investigated for a constant snip of 10 nm, red shift was observed when edge length was increased from 60 nm to 120 nm.

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