Optimisation of Nano Urchin geometry for the generation of hot electrons for sensing: A computational study

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Abstract— **Plasmonic nanostructures are preferred because they raise the Q factor, which improves any device's efficiency. Depending on the geometric structural characteristics of the material, they enhance the absorption of incident light at wavelengths. In this work, we investigate the nano-urchin array's periodic structure on a thin substrate. Additionally, we will investigate the absorbance enhancement that may be utilised in the future to create a sensor for applications like biosensing, photocatalysts etc. that differs in the way that localised plasmons are generated in the cavity created by nano urchin structures.**

Keywords—solar cell, nano particle, periodic array, absorbance, finite difference time domain (FDTD).

I. INTRODUCTION

Surface plasmon resonance (SPR) is a principle that finds application in the majority of sensing applications. These find their use in numerous medical devices across various specialties. One intriguing feature of these sensors is that they are label-free, which eliminates the need for hazardous chemical labels to identify the cells that interact with them and release light, as in the case of the enzyme-linked immunosorbent test (ELISA)[1]. An attractive choice for analyte detection that is based on the localized creation of surface plasmons (LSPRs) produced by asymmetric electron oscillation that have asymmetric structures in the nano-dimension. As a result, there is an electric field enhancement between the structures and hence the term localized. This effect is in use in many biomedical sensing devices that are integrated with microfluidics.[2]. The key difference between the SPR devices and LSPR devices is that the thin films do not show LSPR as the oscillations happens symmetrically on the surface[3].

Periodic plasmonic nanostructures provide a dynamic new insight in light scattering and absorption properties[3]. This is not only limited to metallic nano structure prepared on top of a substrate or a metallic nanohole array sensor[4] but also to materials such as doped graphene nano disks[5], carbon nanotubes[6] etc. These structures provide strong plasmonic resonances and can be used to build a proper sensory device for biomedical application[7]. The field of energy sciences also use a lot of its merits in generation of photo-current (i.e. J_{sc}) [8] as seen in a typical solar cells that are photovoltaic cells containing boundaries of p and n junction. Plasmonic materials are typically employed in semiconductor junctions to restrict light and serve as an antireflective layer for metal oxides. [9] and reflective back layers[10] that are in the bottom of such devices.

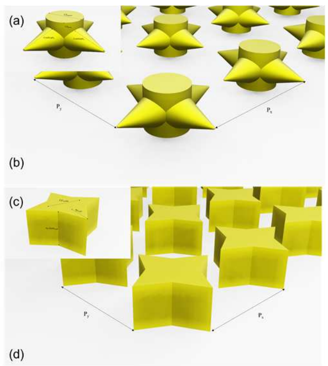

Figure 1: (a)-(b) Schematic diagram of the proposed nano-urchin structure and (c)-(d) the triangle nano stars for comparison. The periodicity mentioned as P_x and P_y with other geometric parameters.

In this work, we offer new perspectives on the numerical computation of the rate of absorbance in the nanostructure, which resembles a nano-urchin (see fig 1 (a-b)), while accounting for variations in geometry and the distances between neighbouring nano urchin (NU) tips, which form an optical cavity where light can be confined. The field is observed to be enhanced, increasing the quality factor. We will talk about the applied methodology of the same including

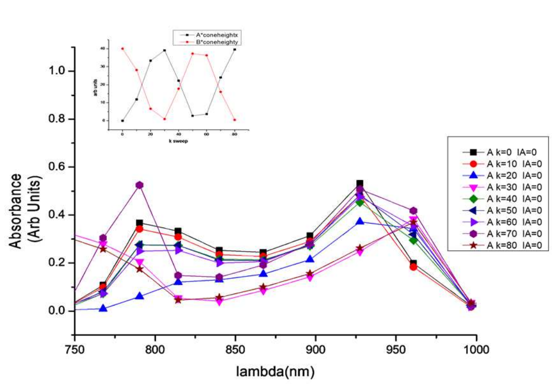

Figure 2: The inset shows the sweep parameter k variation with the cone height. The variation of absorbance of different k values are shown below. This absorbance is of the conical nano urchins (NUS) with cavity size varying in x and y axis. The maximum absorbance at higher energy is seen at wavelength value 790.323 nm at normal incidence (i.e. incidence angle (IA)=0) and k value=70.

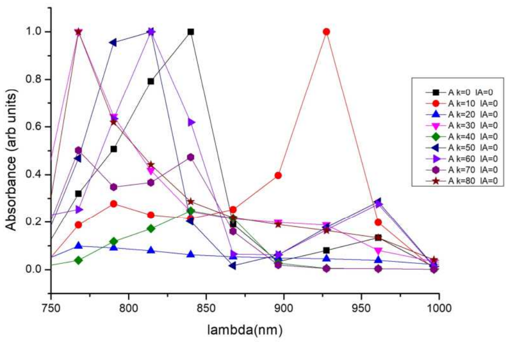

Figure 3: With the same k parameter sweep the absorbance pattern were recorded in nanostars are recorded with highest absorbance at wavelength 767.24 nm and k=80 value.

the geometry and the setup in the application of Lumerical employing the finite difference time domain (FDTD) scheme. Theory

The development of surface plasmon resonance is seen between two boundaries of different permittivity's. Its unique property causes an electron on the medium's surface to resonate inside the material's boundaries between positive and negative permittivity, producing a wave. This is known as the "plasmon- wave"[11]. The condition for the generation of surface plasmons is dependent on the dispersion relation $\beta = k_0\sqrt{\frac{\varepsilon_m \cdot \varepsilon_d}{\varepsilon_m + \varepsilon_d}}$ where β is the wave vector of the plasmon wave, ε_m is the permittivity of the metal, ε_d is the permittivity of the dielectric and $k_0 = \frac{\omega}{c}$ where ω is the angular frequency and c is the speed of light in free space[2]. This phase matching condition is important for the wave to propagate through the boundaries of both the medium. Plasmonic sensors depend on the generation of these trapped oscillation on the surface and particularly the generation of LSPR which depends on the nano width distances between the cavity formed by two tips [7]. One of the interesting parameter to look into is the generation of "hot-electrons" that are more energetic than the Drude electrons[12]. The generation of these hot electrons are given by[13]:

$$Rate_{HE} = \frac{1}{4}\frac{2}{\pi^2}\frac{e^2E_f^2}{\hbar}\frac{(\hbar\omega - \Delta E_b)}{(\hbar\omega)^4}\int_s |E_{normal}|^2 dS \quad (1)$$

Where E_f is the Fermi energy, ω is the frequency, $\Delta E_b$is the Schottky barrier potential energy between semiconductor and metal nanoparticle and E_{normal} is the electric field normal to the surface.

II. Results and Discussions

The development of our model is based on the two primary structures connected to a semiconductor silicon (Si) substrate with a known ΔE_b of around 0.2 ± 0.1 eV[14] and Fermi energy E_f of 5.31 eV [15]. The gold nano cylinders and gold nano stars have been primarily been explored in this area with studies done with optimisation of the structure and their respective periodicity. Here we consider a parameter k that decides the length of a fixed cone height by varying by the following equation:

$$f(k) = (\sin(k))^2 + (\cos(k))^2 \quad (2)$$

This enables us to look into the simultaneous change of the cone height in the x and y axis. The periodicity is kept constant at 150 nm with NU tip distance kept at 10 nm when both the conical tips are unchanged. The generation of the hot electrons using the above mention equation 1 shows that the confinement of light is more in NUs rather than nano stars and the generation of hot electrons are approximately ~2.5 times more than nano stars. Hence in conclusion, the hot electron generation sensing is highly structural dependent as well as the power of the incident photon that uplifts the electrons energy to a higher orbital that can be used for sensing related devices with a high accuracy.

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