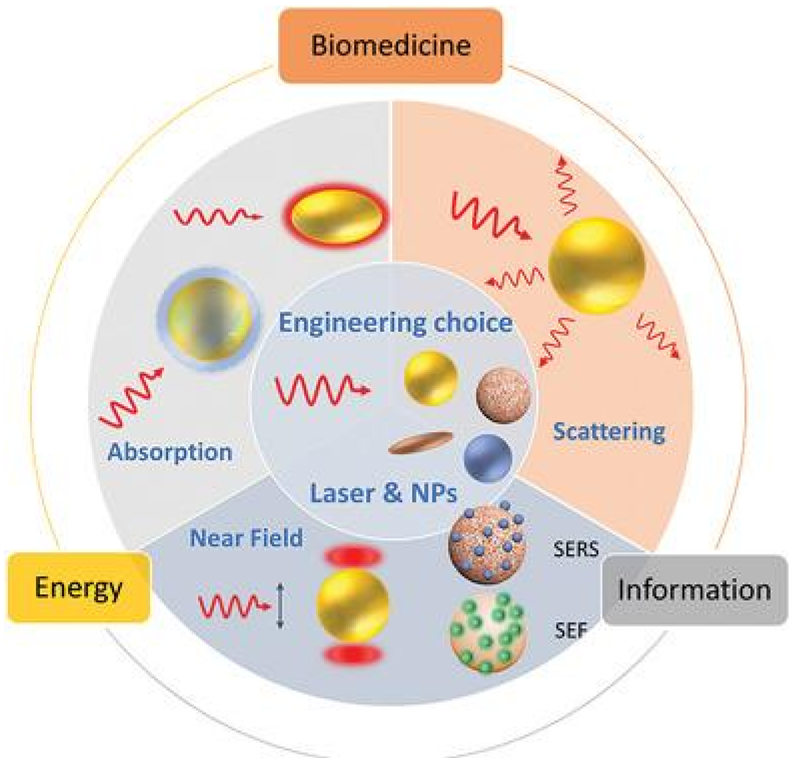
# THESIS

## Modeling of plasmonic property of Nanomaterials of noble metals and it's alloys




**Yash Raj Bharti**

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## ABSTRACT

Metallic, especially gold, nanostructures exhibit plasmonic behavior in the visible to near-infrared light range. In this study, we investigate optical enhancement and absorption of gold nanobars with different thicknesses for transverse and longitudinal polarizations using finite element method simulations. This study also reports on the discrepancy in the resonance wavelengths and optical enhancement of the sharp-corner and round-corner nanobars of constant length 100 nm and width 60 nm. The result shows that resonance amplitude and wavelength have strong dependencies on the thickness of the nanostructure as well as the sharpness of the corners, which is significant since actual fabricated structures often have rounded corners. Primary resonance mode blue-shifts and broadens as the thickness increases due to decoupling of charge dipoles at the surface for both polarizations. The broadening effect is characterized by measuring the full width at half maximum of the spectra. We also present the surface charge distribution showing dipole mode oscillations at resonance frequency and multimode resonance indicating different oscillation directions of the surface charge based on the polarization direction of the field. Results of this work give insight for precisely tuning nanobar structures for sensing and other enhanced optical applications.

Noble-metal nanoparticles have been the industry standard for plasmonic applications due to their highly populated plasmon generations. Despite their remarkable plasmonic performance, their widespread use in plasmonic applications is commonly hindered due to limitations on the available laser sources and relatively low operating temperatures needed to retain mechanical strength in these materials. Motivated by recent experimental works, in which exotic hexagonal-closed-packed (HCP) phases have been identified in gold (Au), silver (Ag), and copper (Cu), we present the plasmonic performance of two HCP polytypes in these materials using high-accuracy first-principles simulations. The isolated HCP phases commonly reach thermal and mechanical stability at high temperatures due to monotonically decreasing Gibbs free-energy differences compared to face-centered cubic (FCC) phases. We find that several of these polytypes are harder and produce bulk plasmons at lower energies with comparable lifetimes than their conventional FCC counterparts. It also leads to the localized surface-plasmon resonance (LSPR) in perfectly

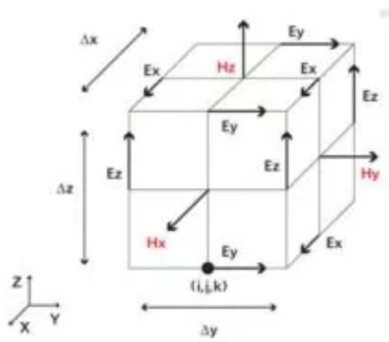
spherical HCP-phased nanoparticles, embedded onto dielectric matrices, at substantially lower energies with comparable lifetimes to their FCC counterparts. LSPR peak locations and lifetimes can be tuned by controlling the operational temperature, the dielectric permittivity of the hosting matrix, and the grain size. Our work suggests that noble-metal nanoparticles can be tailored to develop exotic HCP phases to obtain novel plasmonic properties.

## INTRODUCTION TO FDTD

The Finite-Difference Time-Domain (FDTD) method is a rigorous and powerful tool for modeling nano-scale optical devices. FDTD solves Maxwell's equations directly without any physical approximation, and the maximum problem size is limited only by the extent of the computing power available.

## METHODS

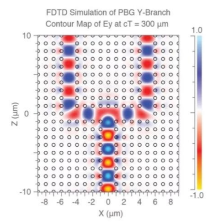
The FDTD method solves Maxwell's equations on a mesh and computes E and H at grid points spaced $\Delta x$, $\Delta y$, and $\Delta z$ apart, with E and H interlaced in all three spatial dimensions. FDTD includes the effects of scattering, transmission, reflection, absorption, etc. FDTD is a time-domain solution, but frequency analysis is also possible through the use of the Fast Fourier Transform (FFT) and the Discrete Fourier Transform (DFT).




*FDTD Yee Cell of dimension Ax, Ay, Az. [3]*

FDTD can simulate any structure where Maxwell's equations describe the necessary physics. Typical applications for this method include: LEDs, solar cells, filters, optical switches, semiconductor-based photonic devices, sensors, nano- and micro-lithography, nonlinear devices, and meta-materials (negative index of refraction). Read about FullWAVE FDTD for details about additional applications.

Synopsys offers several photonic solutions tools that employ the FDTD method.




*FDTD Simulation of Y-branch PBG splitter*

Synopsys' FullWAVE FDTD simulation software, part of RSoft Photonic Device Tools, employs FDTD to perform a full-vector simulation of photonic structures. Its award-winning, innovative design and feature set has made FullWAVE FDTD the market leader among optical device simulation tools, with a cutting-edge implementation of a mature FDTD algorithm that allows for a wide range of simulation and analysis capabilities. For a wide range of integrated and nano-optic devices, FullWAVE FDTD has applications such as LED extraction analysis, diffractive optical element (DOE) design, PIC/Custom PDK element design, nanophotonics, and meta-materials design.

## FullWAVE FDTD Example: Modeling a Surface-Plasmon-Based Spatial Multiplexer

The speed of intra-chip and inter-chip connection is one of the main bottlenecks to achieving faster computer chip performance. Routing the signals through surface-plasmon-based waveguides provides one possible way to achieve faster optical connection speeds; these waveguides are compact, not bound by the diffraction limit, and can be easily integrated with both optical and electronic technologies.

One basic challenge facing the adoption of plasmon guides within electrical chips is the excitation of the plasmons from external sources. Simulating this effect requires a rigorous full-vector modeling environment that provides accurate solutions for arbitrary device geometries containing both metallic and nonmetallic components. FullWAVE FDTD is the ideal tool to meet this need. FullWAVE provides a full-vector solution to Maxwell's equations and allows engineers to use complex material definitions, arbitrary device geometries, non-uniform grids, and sophisticated measurement techniques to create new plasmonic devices and fine-tune existing designs for specific applications. The design parameters of the structure can also be perturbed in FullWAVE FDTD to allow the study of manufacturing tolerances on device performance.

The surface-plasmon-based spatial multiplexer studied in Figure 1 consists of a multiplexing switch that steers light toward one of several subwavelength metal-strip waveguides. Several 3D FullWAVE FDTD simulations were performed at a fixed wavelength, at various incident angles of the illumination to determine the optimal angles at which light is coupled into each of the three metal-strip waveguides.

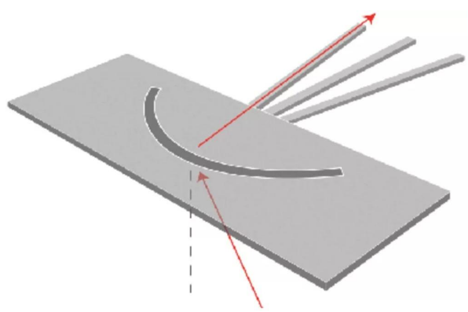


*Figure 1: Schematic of the surface-plasmon spatial multiplexer*

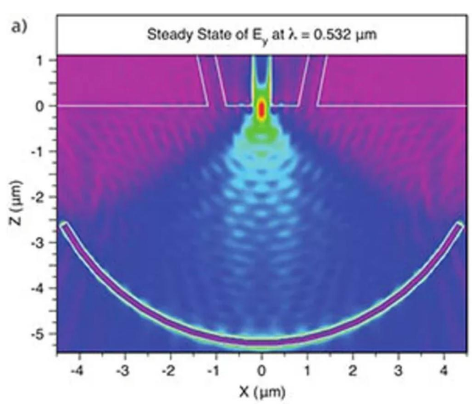



*Figure 2: Simulation results showing the amplitude of the Ey field on the surface of the metal film:*
*a) Normal incidence light (shown above) is coupled into the central metal-strip waveguide*
*b) Angled incident light is coupled into one of the side metal-strip waveguides*

## APPLICATIONS

Efficient Radial FDTD Calculation in RSoft Photonic Device Tools

Creating a Pulse Train in FullWAVE FDTD Using Custom Time Envelopes

Simulation of a Dielectric Q-Plate for Millimeter-Wave Photonic Orbital Angular Momentum Applications.

## CONCLUSION

In this study, plasmonic properties of gold nanobars with various thicknesses were computationally analyzed. Sharp-corner and round-corner rectangular nanobars were studied; comparisons of the peaks the spectra reveal that the round-corner nanobars shows an average of 30 nm shift to lower wavelength for the same size for both incident polarization. Resonance peak wavelengths shifted toward blue for both absorption and enhancement spectra with increasing thicknesses due to decoupling of the charge dipoles on the top and bottom surface. As the thickness increases, the FWHM of the spectrum also increases due to the impact of higher order modes which have been visualized in our surface charge density distribution calculations. The results reported here are significant for plasmonic structures fabricated with electron beam lithography since we investigate key fabrication parameters including thickness of the nanobars and round corners, a property of nanostructures fabricated with method.

The use of surface plasmon resonances in chip interconnects can allow for much faster chip performance. As shown in this example, rigorous simulation software like FullWAVE FDTD provides the necessary tools to study all factors that contribute to the design of a surface plasmon device.

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