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Simulation Environment for Optimized Grating-Based Plasmon Couplers

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Summary:
The properties of surface plasmons create the potential for sensitivity to nanoscale environmental changes and allows for practical applications including light guiding, nanomanipulation, biosensing, high-resolution imaging, and optical switching. Grating structures have emerged as a central tool enabling the design of dedicated systems for modulating light-matter interactions. This contribution presents a Finite-Difference Time-Domain (FDTD) method enhanced with the Drude model, Perfectly Matched Layer, Periodic Boundary Condition, and Total Field/Scattered Field-Method that form the basis a simulation environment for surface plasmon couplers. The simulations are able to cover a wide parameter space, aiding optimal design identification. Validation against experimental results on actual grating structures has been used to improve the model's accuracy and predictive capabilities. This iterative approach yields insights into efficient grating-based plasmon coupler designs thus contributing to plasmonics understanding and optimized applications.

Keywords: Surface Plasmon, Grating, Simulation, FDTD method

Introduction

Surface plasmons are coherent oscillations of electrons at the interface of a metal and a dielectric substance. They feature unique properties that have driven significant research and development in a multitude of sensing applications. Their high sensitivity in local environments at the nanoscale has enabled a wide range of practical applications. Among the various techniques to harness these properties, grating structures have emerged as a crucial tool for controlling and enhancing the interaction between light wave and matter. They are of particular interest when aiming at designing integrated microdevices and tailoring device performance to specific applications.

The performance of grating-based plasmon couplers crucially hinges on the excitation angle of plasmonic modes. Both the size and thickness of the grating elements are known to impact the excitation angle, affecting the coupling efficiency and overall device functionality [1]. The relationship between these parameters, the materials used in grating fabrication, and the resulting excitation angle is complex and requires a comprehensive understanding to design optimized plasmonic couplers.

The Finite-Difference Time-Domain (FDTD) method [3], which is a numerical simulation technique widely used to model electromagnetic wave propagation and interaction with complex structures is deployed to accomplish this task in an efficient manner. To achieve an accurate representation, the Drude model method, Perfectly Matched Layer (PML), Periodic Boundary Condition (PBC), and Total Field/Scattered Field-Method (TF/SF) are included into the simulation environment. This computational approach allows for rapid exploration of a wide parameter space, facilitating the identification of optimal grating designs for specific plasmonic applications [4].

Simulation Environment

The simulation environment has been designed to accurately predict the behaviour of actual grating structures with high efficacy at optimzed computational costs. To this end, appropiate adjustments and boundary conditions have been implemented. The model presented here has been used to guide and validated grating designs via comparison to experimental results using a silver-based grating coupler [5].

To derive the governing equations for the 2D case in the x-y-plane, only the TM mode with the electrical field components E_x, E_y, the magnetic field component H_z and polarization current density components J_x, J_y are considered. The approximation is formed at a location between the neighbouring components but not at the location of the points themselves. This procedure is as well valid for the time derivatives for which the midpoint between the time steps n and $n+1$ is taken. The spatial discretization pattern is illustrated in Figure 1.

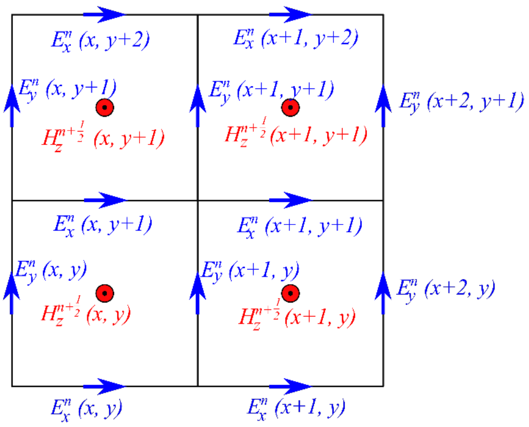

Figure 1: Representation of the Yee grid: The electric and magnetic field values are shifted against each other by half a time step in order to produce results that are possible physical solutions accurately describing the system behaviour.

For the analysis of the behavior of electromagnetic fields at thin metal layers, the Drude model is implemented and the excitation of the incident wave is performed using the Total Field/Scattered Field (TF/SF) method. 2D simulations with periodic boundary conditions are used to analyze the structure's behavior. The structure of the simulation area is shown in Figure 2.

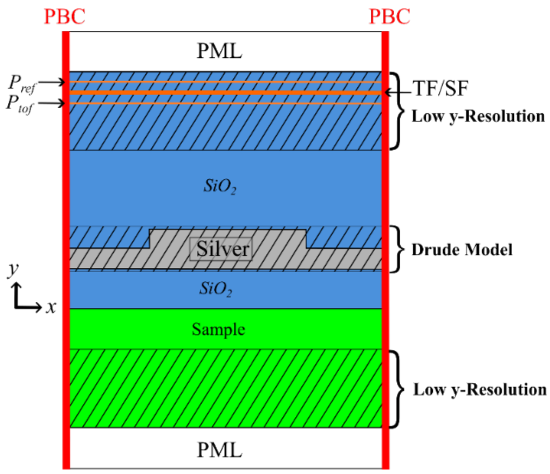

Figure 2: Structure for validating the chosen model indicating the areas of the PLM and periodic boundary condition as well as for the TF/SF method. The Drude model is implemented for the Plasmon excitation region, taking into account the realities of the fabrication process.

Results

The simulation model yields good agreement with experimental results. An exemplary analysis of the effect of changing the simulation resolution in the x-direction is investigated. For this purpose, reflectance spectra are calculated for different discretization widths Δx. The results are shown in Figure 3.

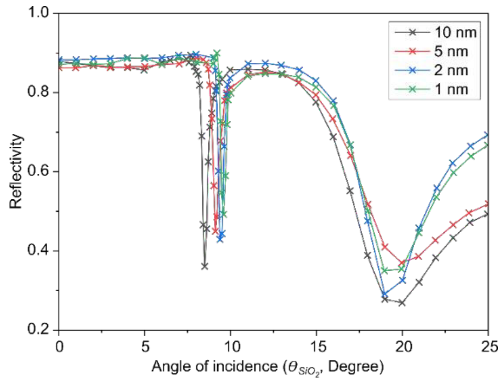

Figure 3: Simulation of the described structure under variation of the resolution in x-direction. The resolution in y-direction is 2 nm, the thickness of the dielectric layer is 1100 nm and the PML is 50 points wide. A pronounced influence on the accuracy of the simulated results with the simulation resolution may be appreciated.

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