Title: Quantitatively Engineering Surface Plasmon Coupling Through Computer Simulation

Authors: Daniel P. Ceperley, Andrew R. Neureuther

Surface plasmons play an important role in many emerging optical devices; however, quantifying their effects on device performance is difficult. We demonstrate a novel means of quantifying surface plasmon generation efficiencies in grating-based devices through a combination of signal flow graphs and Finite Difference Time Domain (FDTD) simulations. We have extended our FDTD simulation capabilities to create a Device Under Test (DUT) system which we utilize to accurately measure surface plasmon coupling efficiencies in the presence of strong low-angle radiation while keeping FDTD simulation sizes to a minimum. We demonstrate the methodology on two devices: 2D nano-wire gratings and Daguerreotypes (arrays of nano-particles).

FDTD is a good method for assessing device performance because it directly solves Maxwell's equations and so includes all the physics. However, it is difficult to assess the impact of individual phenomena, such as surface plasmons, with FDTD precisely because it simulates all phenomena together [1]. Consequently, we us FDTD to measure scattering cross-sections for isolated grating elements and then construct a full-grating signal-flow model based on these cross-sections (Fig. 1). In addition to providing simplified device models, signal flow graphs enable rapid probing of geometrical design levers, such as inter-wire spacing.

Accurately measuring surface plasmon strength is complicated by low-angle radiation which coherently interferes and masks surface plasmons. Spectrally isolating surface plasmon peaks with Fast Fourier Transforms (FFT's) requires large simulation windows, up to 50λ wide, with large simulation runtimes and memory requirements. Scattered wave decompositions use geometrical arguments to significantly reduce the simulation window size and suppress low-angle radiation (Fig. 2). However, this method requires taking the difference between simulations of three different geometries: grating element only, smooth metal surface, and the full geometry (which includes both the grating element and the smooth surface). Using these methods we have found that FFT methods can underestimate surface plasmon peaks by 2x.

The Daguerreotype is a photographic process first demonstrated in France in 1838 utilizing silver-coated plates [2]. Image contrast is driven by nano-particles that form on the silver surface during development. We use our signal flow/FDTD methodology to quantify the contribution of surface plasmon mediated inter-particle coupling in the image formation process. We have found that nano-wires can be quite efficient surface plasmon generators, with one-directional effective lengths of 40% of the physical length. Height is a critical determinate of effective length and doubling a Silver nano-wire's height from 100nm to 200nm increases its effective length by 2.6x.

[1] A. Neureuther, et. al., "Modeling and simulation for nanometrics," JVST B 23(6), 2005.
[2] M. Barger and W. White, The Daguerreotype, Johns Hopkins University Press, 1991.

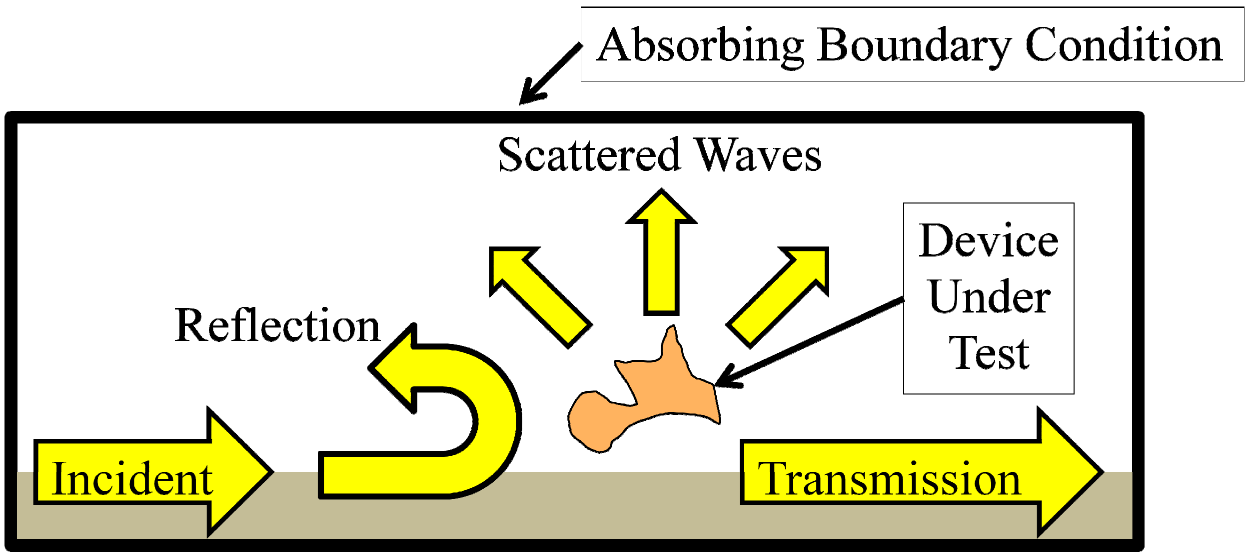

Figure 1: Device Under Test FDTD simulation layout example. A grating element is isolated with absorbing boundary conditions and illuminated with a surface plasmon source. Quantifiable scattering phenomena include surface plasmon reflection and transmission and free-space radiation.

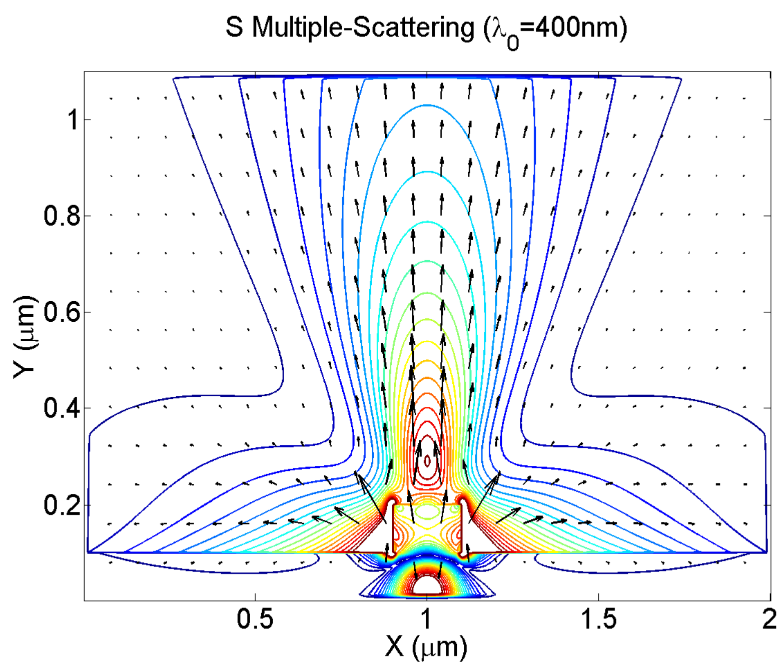

Figure 2: Multiply-scattered power flow around a 200nm wide by 100nm tall Silver bar on a solid Silver substrate (400nm wavelength) produced by plane-wave illumination. By taking the difference of multiple simulations we isolate the fields that have interacted with both the bar and the substrate, which contain all the surface plasmons and less low-angle radiation that hides surface plasmons.