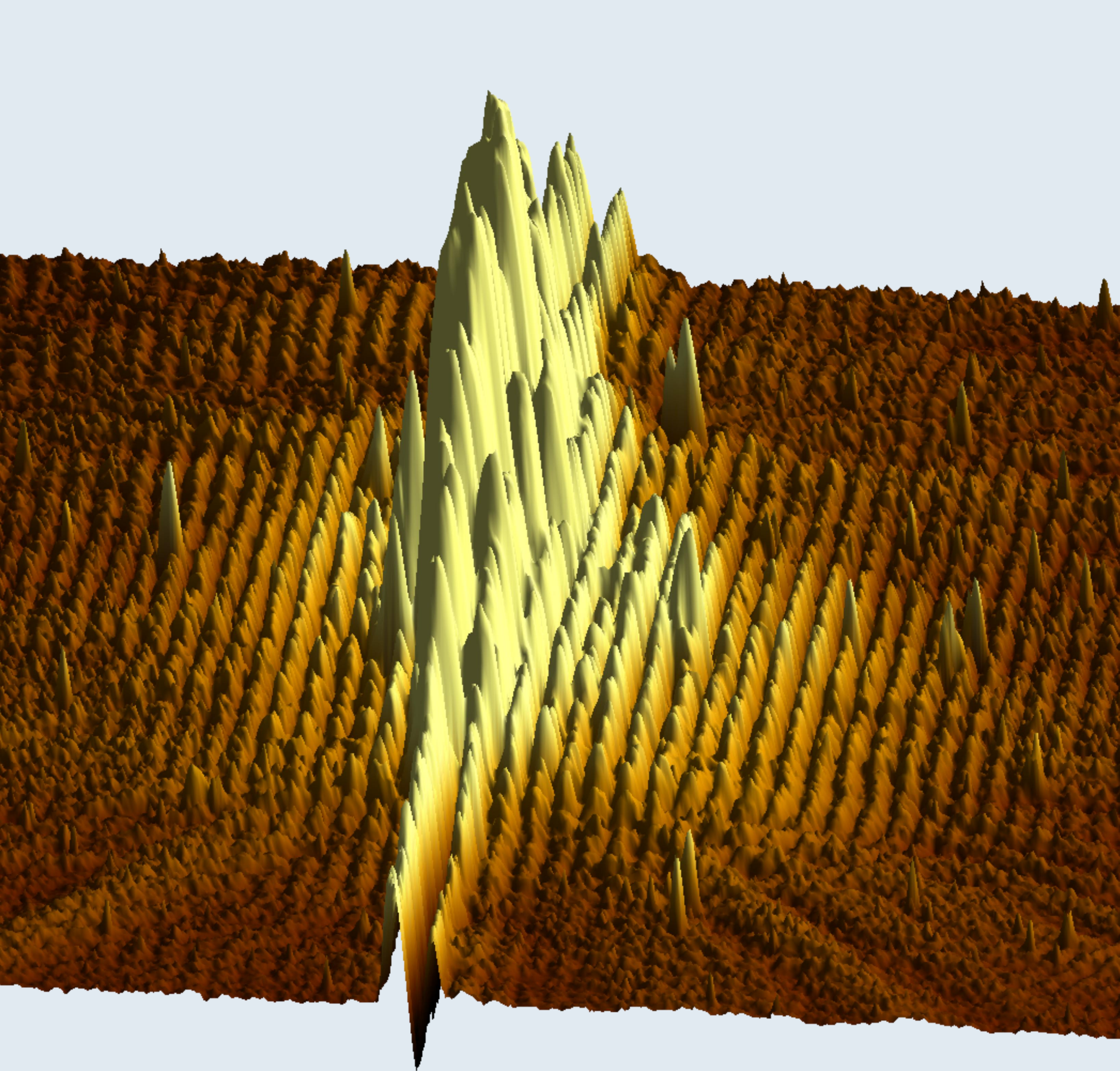




# Simulation and Optimization of Plasmon-Driven Polymerization at Metal–Dielectric Interfaces

Optimization of sample properties for efficient coupling of light to propagating surface plasmon polaritons (pSPPs) and driving the polymerization of diazonium salts<sup>1</sup>.

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## Introduction & Goal

We excite propagating surface plasmon polaritons (pSPPs) by illuminating a nanogroove in a metal film with a laser. The interference with the transmitted light creates an intense standing electric near-field distribution at a dielectric metal interface. We use this distribution to drive the polymerization reaction of diazonium salts. This reaction leads to the formation of a surface relief grating (SRG), which retains the properties of the plasmonic field during irradiation.

We use COMSOL Multiphysics® to simulate these structures to better understand the driving parameters. Furthermore, we aim to optimize crucial parameters of our system, such as layer height, groove width, and propagation length, to improve polymerization efficiency.

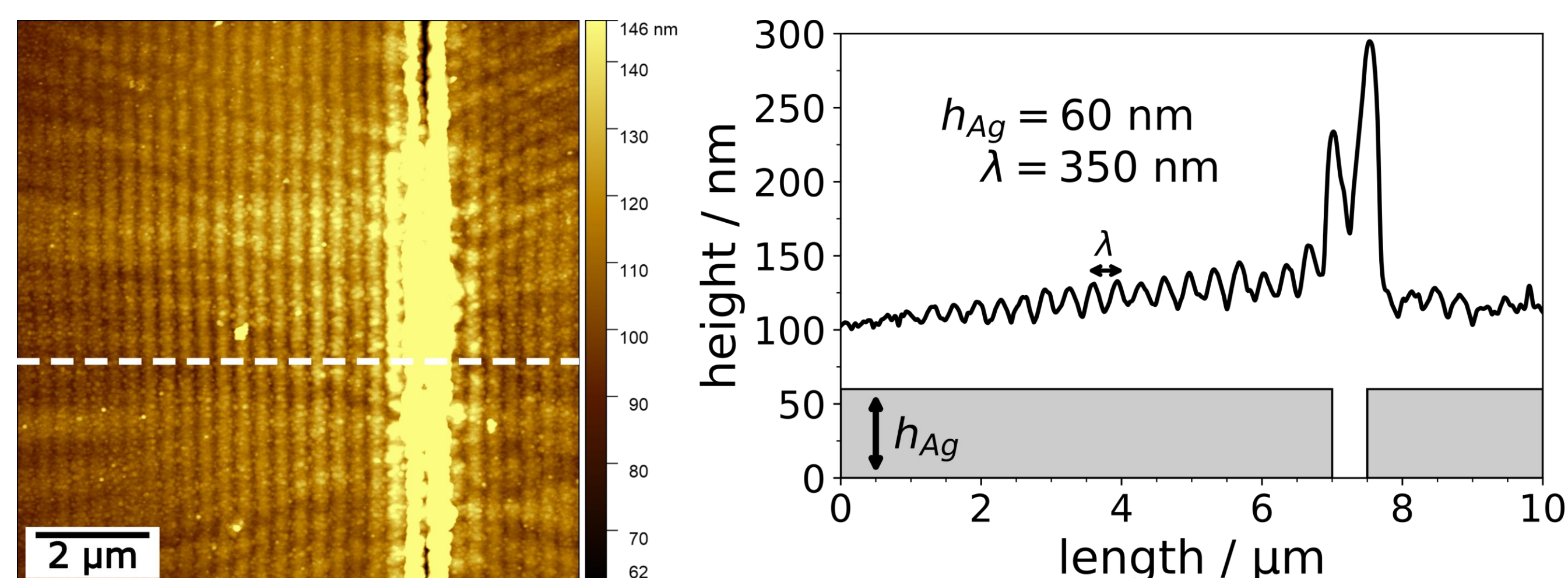


Figure 1. AFM Image of polymerized Diazonium salt by the near field of surface plasmon launched at a silver nanostructure<sup>3</sup>.

## Methodology

We used a two-dimensional (2D) EWFD-simulation to recreate and optimize our experimental system. We simulate a 60 nm silver layer with a 200 nm wide nanogroove in the center. Below we set a glass substrate and on top a 300 nm polymer layer. The excitation laser is simulated by a gaussian scattering condition with electric field polarization perpendicular to the groove.

By adding numerous ports and utilizing the momentum vector of the plasmon, we can calculate various properties such as the coupling efficiency, plasmon wavelengths, and propagation length.

Figure 2 shows the electric field distribution (top), coupling efficiency (bottom left), and propagation length of our simulation.

## Results

The utilization of COMSOL Multiphysics® enabled the simulation of the electric field distribution of the surface plasmon during the polymerization process (See Figure 2, top).

The simulated field aligns well with the resulting SRG structure of the polymer, as shown in Figure 1. The simulated values for plasmonic properties, such as wavelength and penetration depth, fit very well with the values determined experimentally and analytically. However, the values for coupling efficiency and propagation length differ from previous calculations<sup>2</sup>.

In the future, we plan to implement the Optimization and Heat Transfer Modules to improve our simulations and gain a more detailed understanding of the polymerization reaction processes.

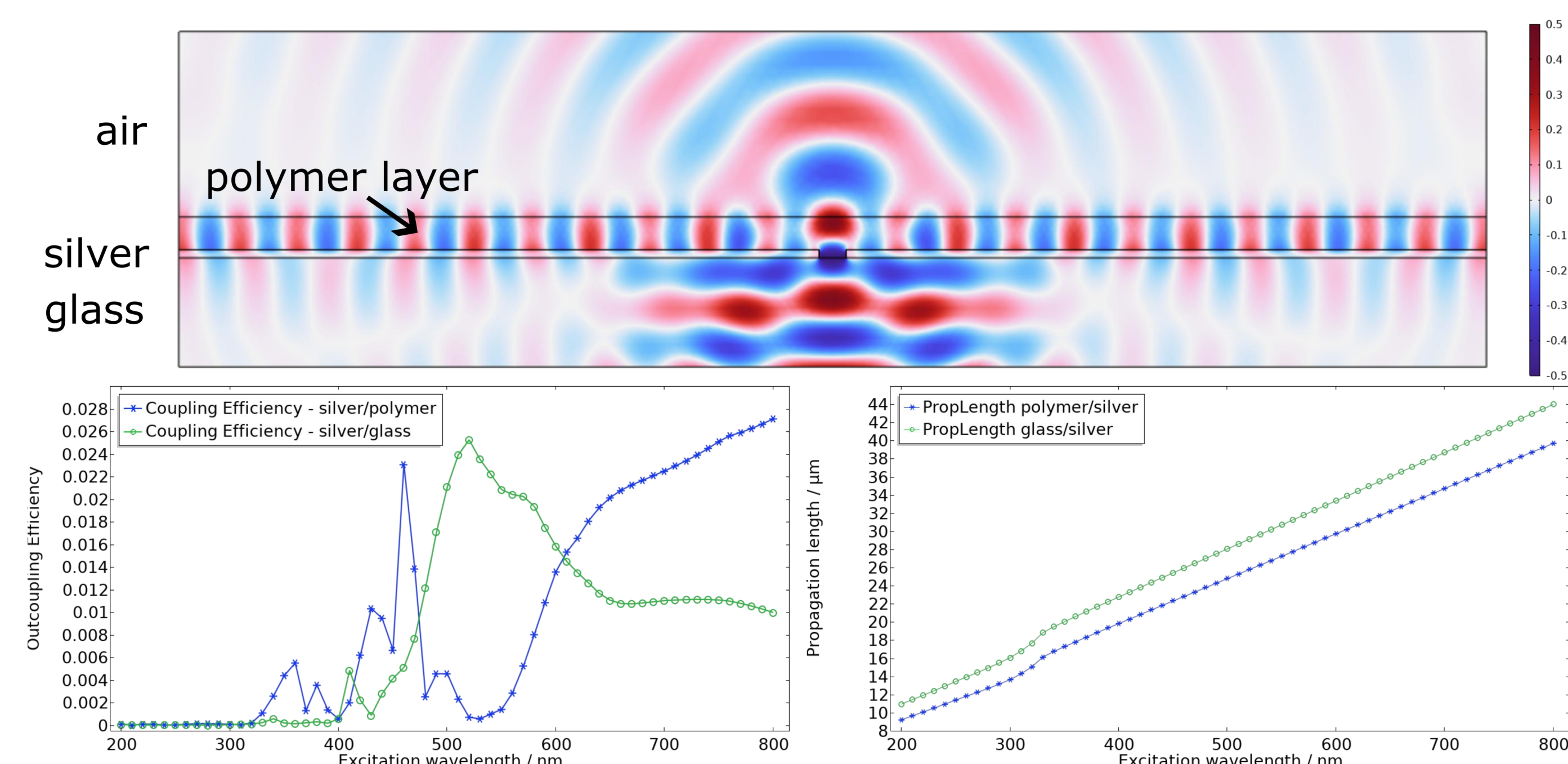


**Figure 2. Top:** Electric field distribution at a thin glass/silver/polymer sample. **Bottom:** Surface Plasmon Properties

## REFERENCES

1. J. Pinson and F. Podvorica, "Attachment of organic layers to conductive or semiconductive surfaces by reduction of diazonium salts," *Chem. Soc. Rev.*, vol. 34, no. 5, pp. 429–439, Apr. 2005
2. T. Papke, N. S. Yadavalli, C. Henkel, and S. Santer, "Mapping a Plasmonic Hologram with Photosensitive Polymer Films: Standing versus Propagating Waves," *ACS Appl. Mater. Interfaces*, vol. 6, no. 16, pp. 14174–14180, Aug. 2014
3. G. Stockmann, et .al., Surface-Confined Polymer Growth Guided by Plasmonic Near-Field Interference, in preparation

