Study of the Optical Field Scattering Enhancement on a 2D Rough Surface using COMSOL Multiphysics®

De Carvalho Gomes, Paulo[1], Goldberg Oppenheimer, P. [1]
1. School of Chemical Engineering, University of Birmingham, UK

OUTLINE: In the introduction, we give an overview of the microfabrication steps to produce our patterned surface. After the patterned formation, the pattern is characterized and, based on the characterization, a model of the surface is created on COMSOL®. The goal of this study is to obtain the optical properties of the pattern surface thus we will compare the incident electromagnetic field with the scattering field from the surface. Hence, we aim to optimize the scattering field enhancement by testing different surface patterns. We conclude this poster with the major contributions to the scattering field enhancement.

INTRODUCTION: Study the influence of surface roughness on the scattering field. The roughness is formed on top of the pillars during the Electrohydrodynamic (EHD) process. This roughness can be controlled by a patterned top electrode.

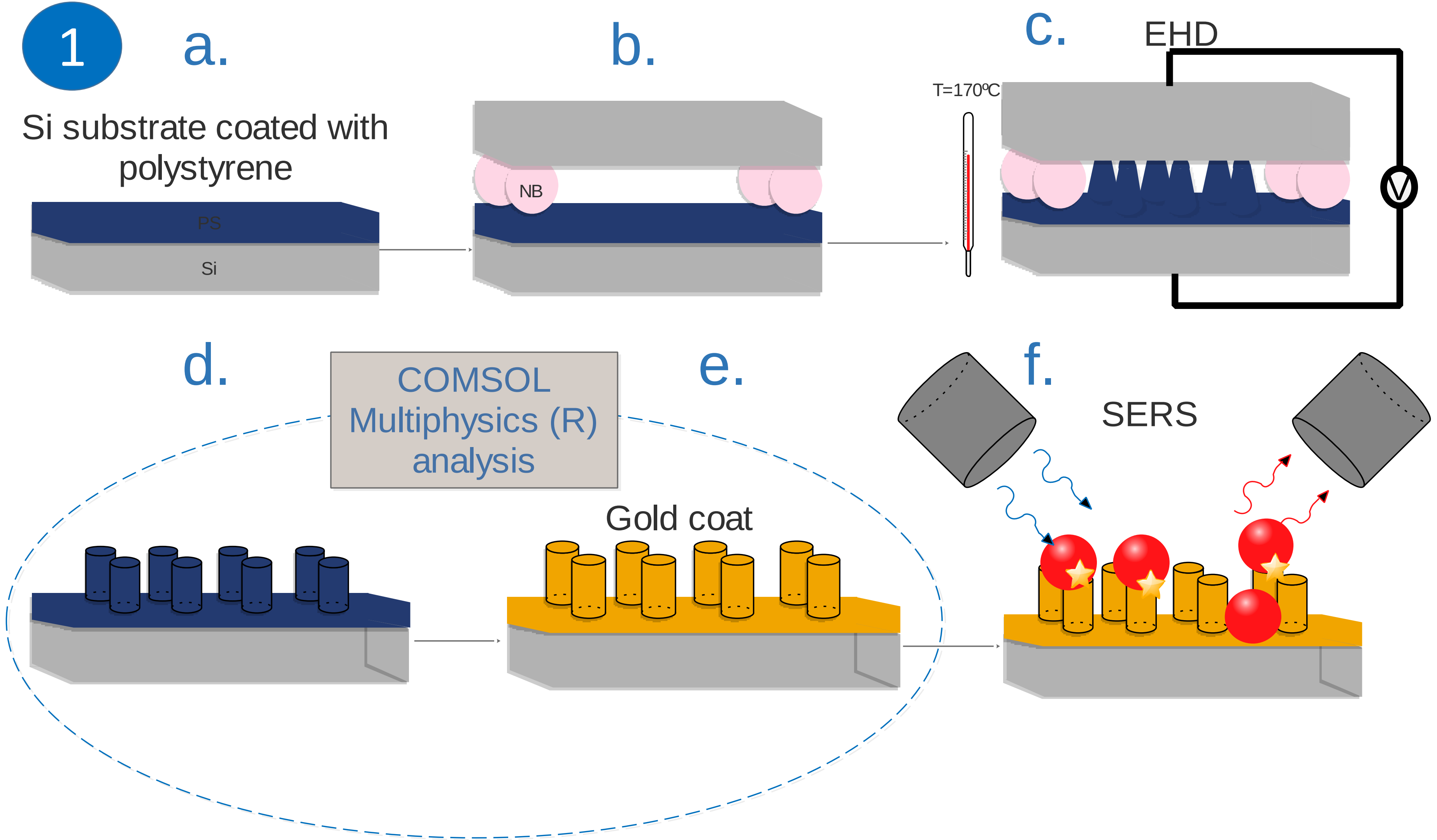


Figure 1. a.-c.: EHD fabrication steps of the patterned surface. **d.-e.:** Patterned surface to be analyzed. **f.:** The final goal of the patterned surface.

This 2D surface is modeled after the topology obtained from the AFM and optical microscope characterization. And later used in the scattering filed simulations.

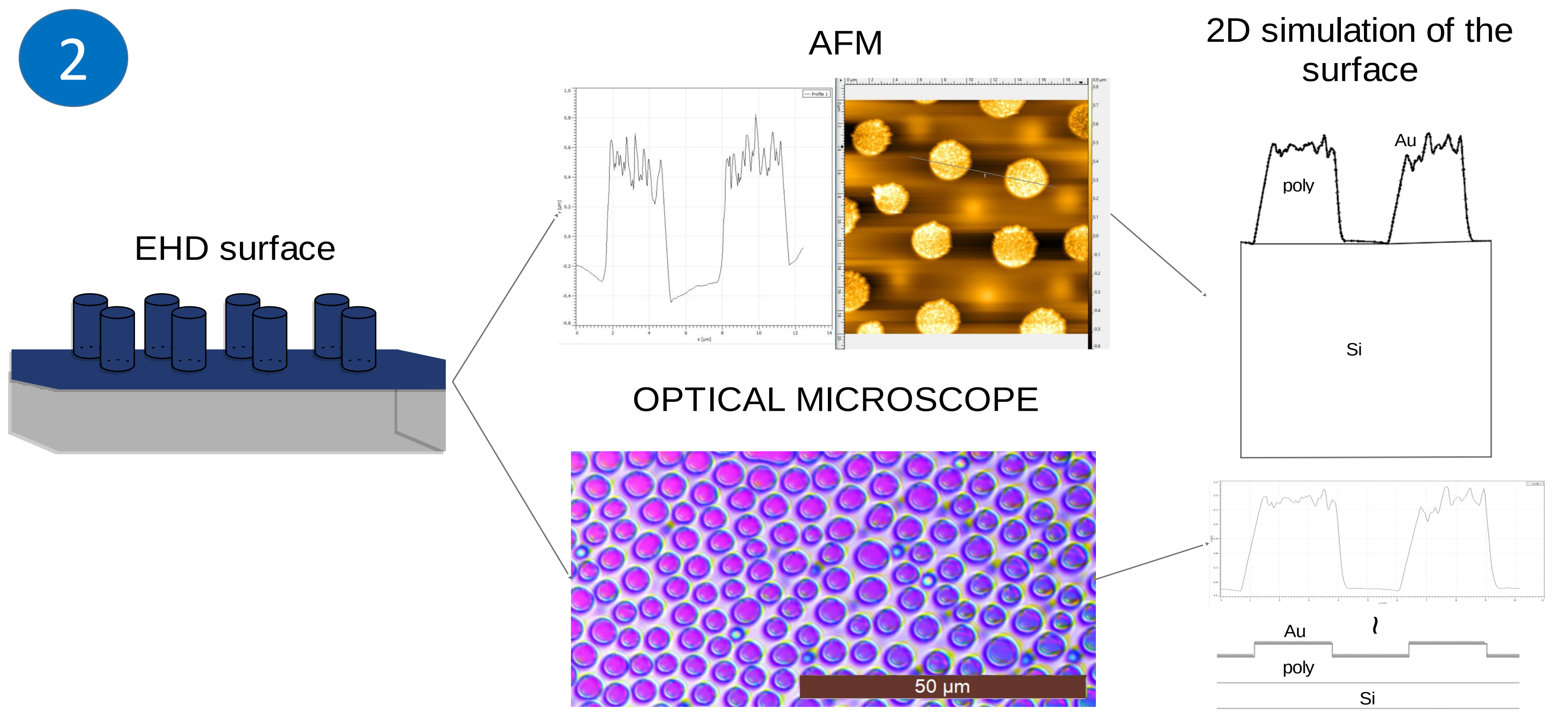


Figure 2. From reality to simulation: AFM and OM characterization of the surface followed by the creation of a surface model.

COMPUTATIONAL METHODS: The method to compute the scattering field from a 2D surface by using the Electromagnetic Waves in the frequency domain – Wave Optics module with PML and SBC:

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{E})-k_0^2\mu_r\left(\varepsilon_r-j\frac{\sigma}{\omega\varepsilon_0}\right)\vec{E}=0$$

Electromagnetic waves, frequency domains

$$\vec{n}\times\left(\vec{\nabla}\times\left(\vec{E}+\vec{E}_b\right)\right)-jk\vec{n}\times\left(\vec{E}\times\vec{n}\right)=0$$

Scattering boundary condition

$$\vec{E}_b=E_0\exp\left(j\frac{2\pi x}{\lambda}\right)\vec{e}_y$$

Background Electric field

RESULTS: The maximum enhancement was obtained when considering a 20 nm roughness size with -10 nm spacing between roughness sites. This patterned gave an enhancement of ~10^7.

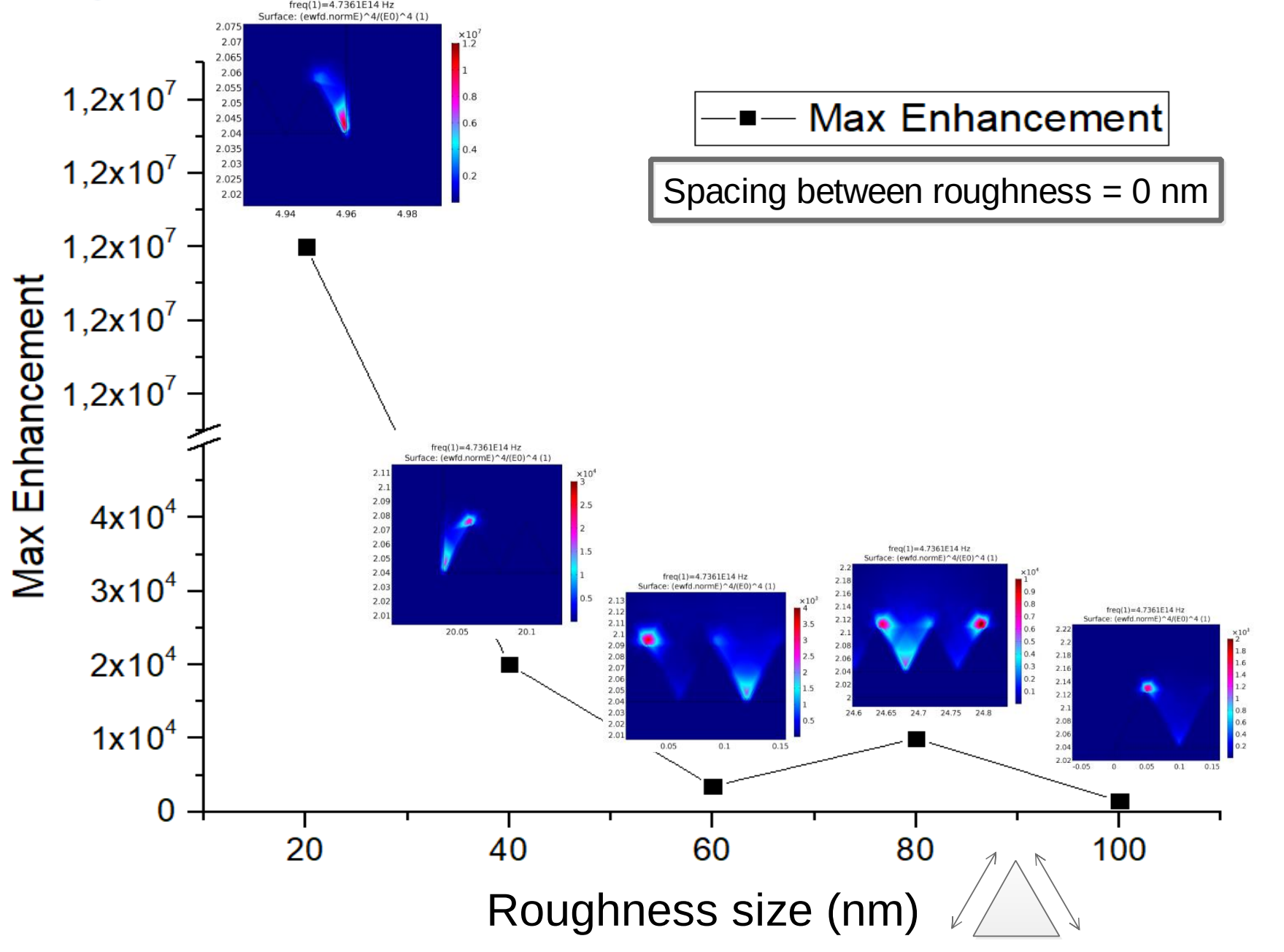


Figure 3. Enhancement vs. roughness size – small roughness size -> bigger enhancement.

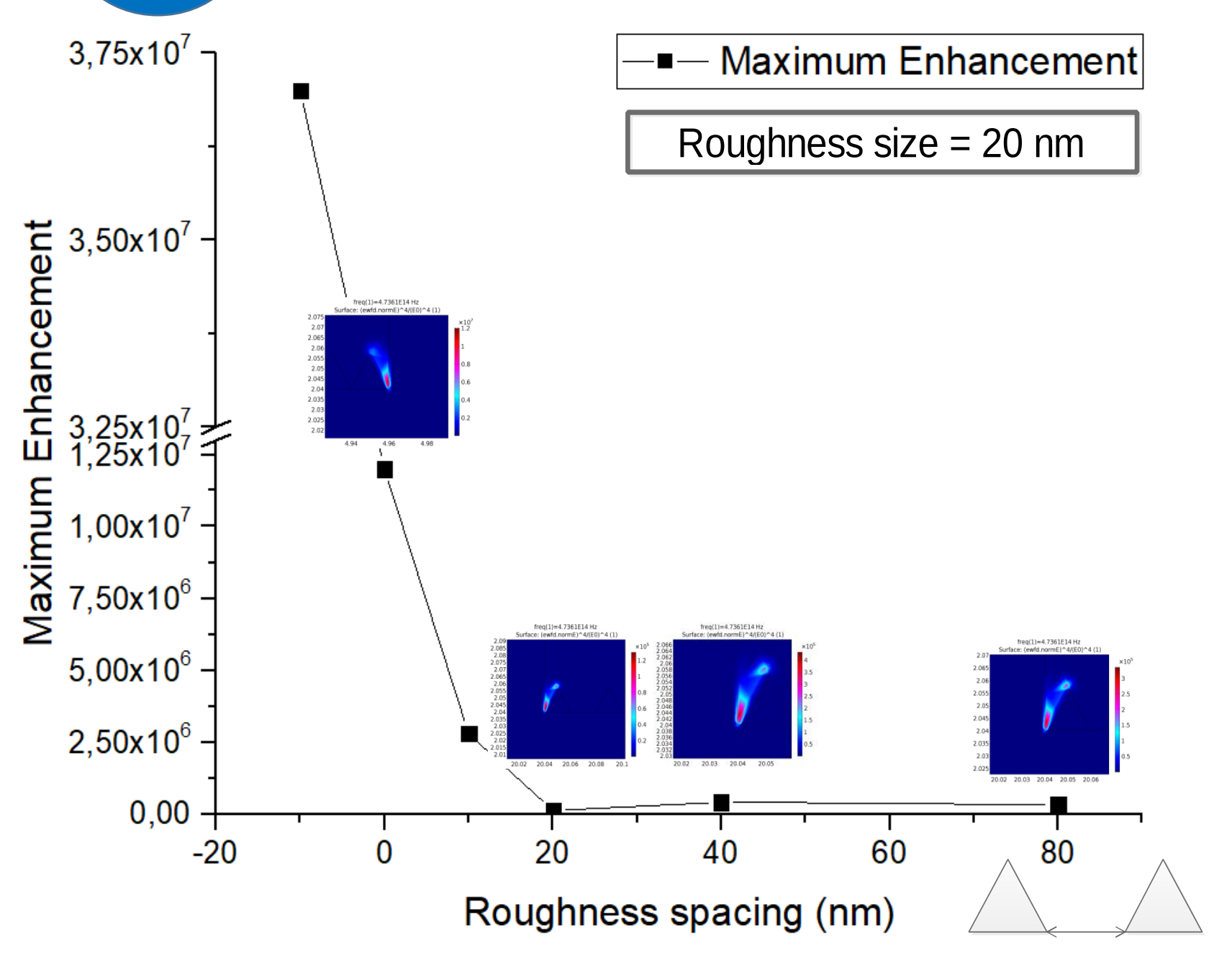
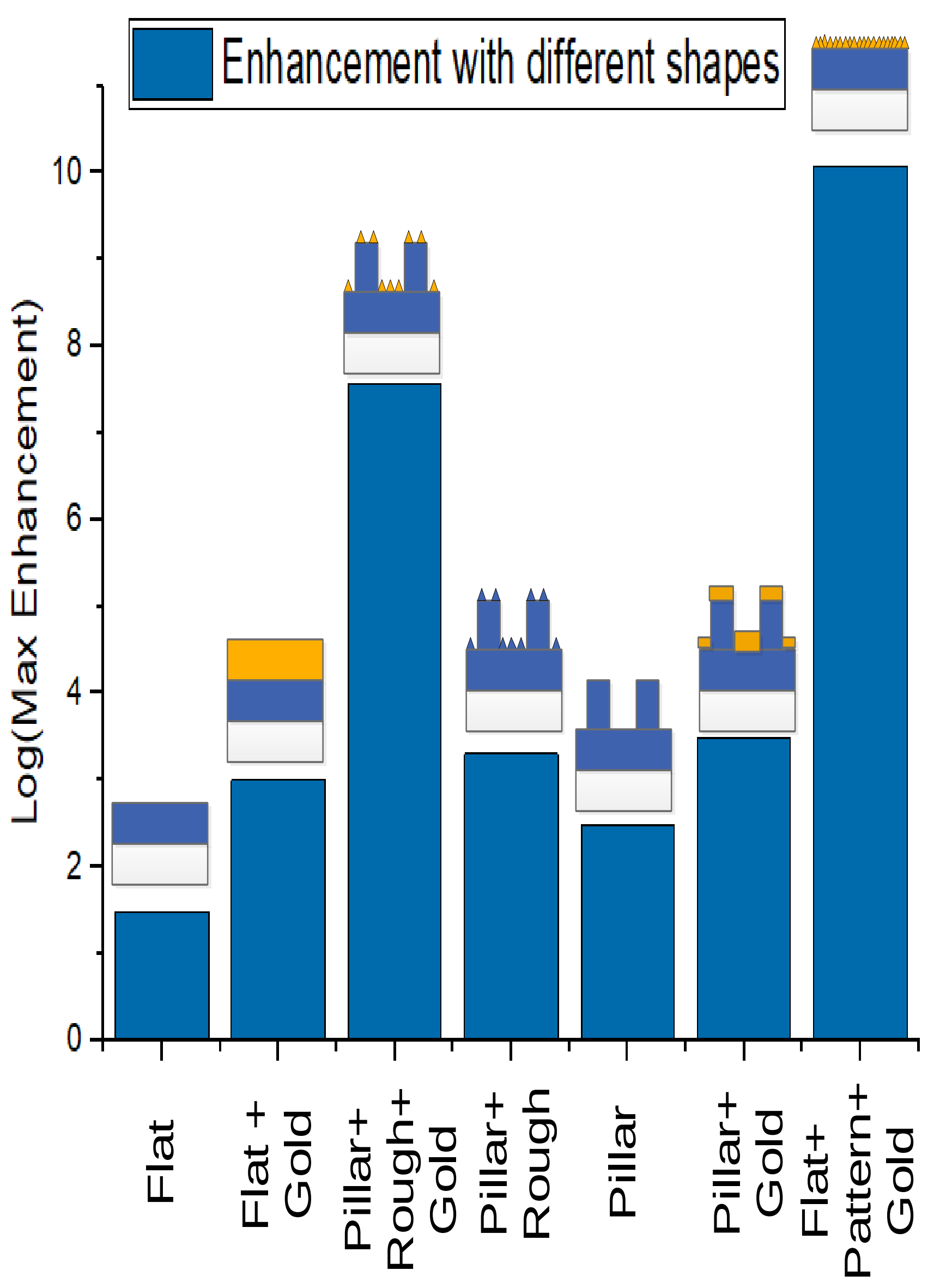


Figure 4. Enhancement vs. roughness spacing – small roughness spacing -> bigger enhancement.

For the best pattern simulation on flat surface, we obtained best results for pattern size equals 640 nm and spacing -320 nm, with an enhancement of ~10^{10}.



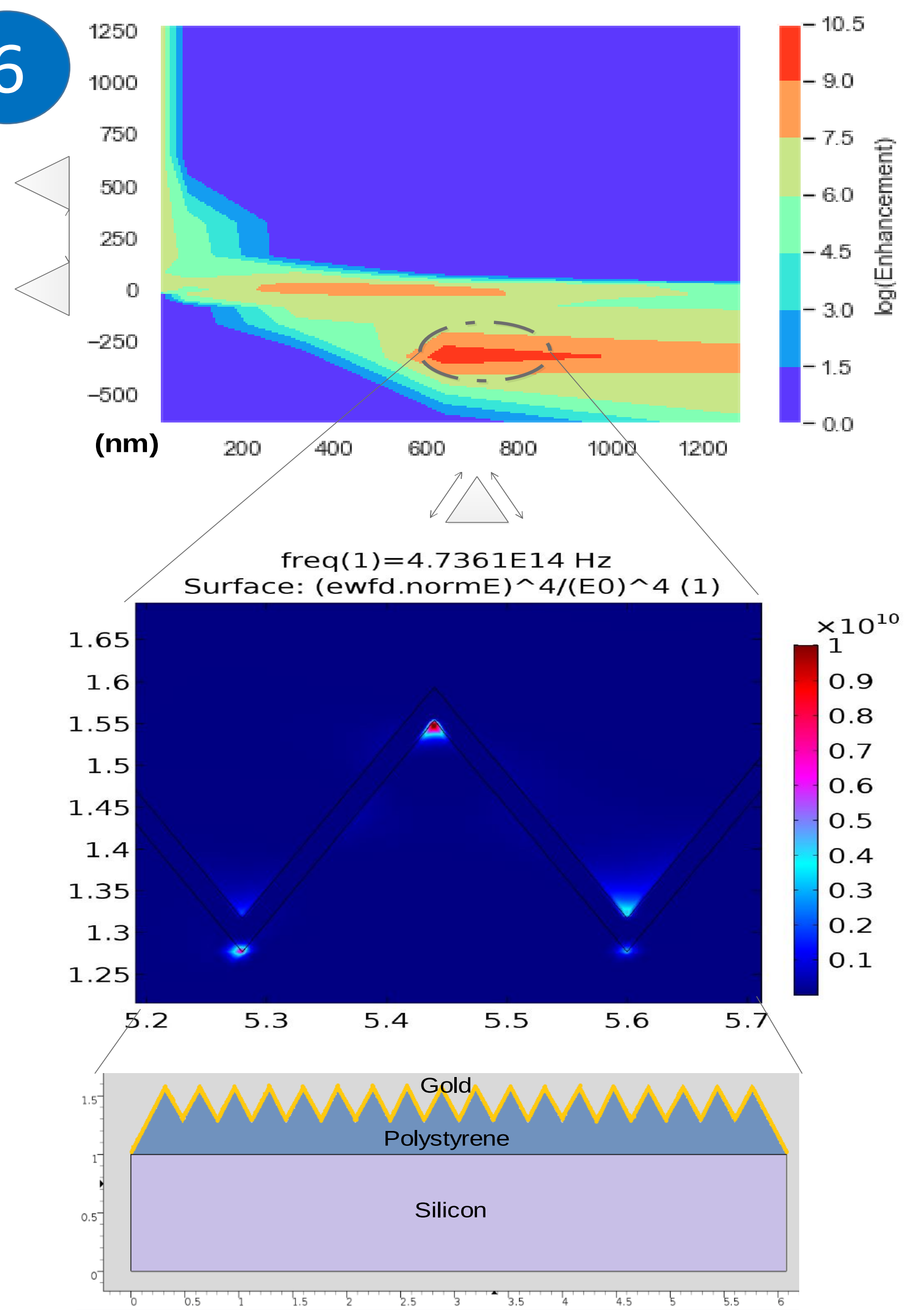


Figure 5. Enhancement comparison between different patterned shapes.

Figure 6. Enhancement 2D plot for all data points. Reference to the max enhancement region.

CONCLUSIONS: The enhancement comes from the confined space between patterned sites or the edge of a roughness site. The best results were obtained for a triangular patterned gold surface. These finding will help us design the optimal surface for our SERS device.

REFERENCES:

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2. Rickard, J. *Et al*, Tunable Nanopatterning of Conductive Polymers via Electrohydrodynamic Lithography, ACS Nano, 2016, 10, 3865-3870

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