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

Abstract

Surface Enhanced Raman Scattering (SERS) phenomenon is well known for its detection sensitivity, however, to better understand how it works a better insight needs to be developed on the physics behind the phenomenon. The physical aspects known to produce SERS effect are the use of coinage metal surfaces with an extremely small roughness over the surface, which when a laser light interacts with these sites, it induces a localized surface plasmons (LSP) that makes the enhancement effect highly localized and strong.

Our group approaches the SERS effect in the following way, we produce a polymeric surface using a technique called Electrohydrodynamic (EHD) Lithography, where a capacitor geometry is used, with top and bottom capacitors made of silicon. The bottom electrode is coated with a thin polystyrene solution and a gap between the two electrodes is made for the polymer to grow in between the capacitors. When current is passed through the capacitor, it exerts electrostatic pressure on the polymer, which will stretch it into a more thermodynamically stable configuration, thus producing micrometer size pillars. Afterward, the pillars are characterized by Atomic Force Microscopy (AFM) and optical microscopy (OM) and the structure is reproduced in COMSOL program for further computations.

When using SERS as a label-free detection substrate, the device lacks reproducibility in the Raman spectra obtained, where from trial to trial, on the same sample, the spectra slightly changes. This is a problem if we want to introduce the SERS technique as a standard procedure in a medical setup where all the measurements, in the same conditions, need to be consistent.

Thus, our objective is to approach the reproducibility issue by focusing on controlling the roughness design and take advantage of the roughness to consistently detect analytes with the same reproducible enhancement factors and Raman spectra. In order to understand how to improve the SERS enhancement with different surface roughness, a COMSOL study was developed where we try different enhancement patterns and check for the maximum enhancement obtained.

The problem was set up in the following way: simulate the roughness of the surface in COMSOL by introducing a 2D surface made of nanometer-sized triangles on top of a flat surface. Afterward, apply an electromagnetic waves physics frequency domain study on

COMSOL to analyze the interaction of the field on the surface. Use perfectly matching layers and scattering boundary conditions to close the system. Finally, solve for the optical field in our given geometry.

Obtained results show that the enhancement comes from the roughness on the surface. The best enhancement comes when the roughness is in a confined space with coinage metal surfaces. The enhancement might appear on top of the roughness or in between roughness spots both called hot spots. When compare with flat surfaces and surfaces with roughness but without the polymer pillars, both configurations gave very small to no enhancement.

Figures used in the abstract

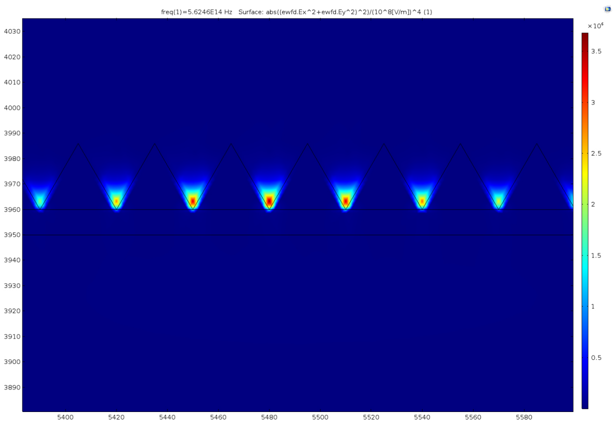

Figure 1: Scattering field enhancement on a gold rough surface (the roughness is simulated by introducing nanometer size triangles in a flat surface). The enhancement on the surface is shown with bright colours that appear in between roughness sites. The enhancement is calculated by the ratio of the absolute value to the fourth power between the scattering field and the incoming field.