ABSTRACT

OPTIMIZATION OF SERS-ACTIVE GOLD SUBSTRATE FABRICATION WITH 4-MERCAPTOBENZOIC ACID MODIFICATION FOR ENHANCEMENT FACTOR

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This research investigates the enhancement of localized electric fields in inverted-pyramidal gold (Au) nanostructures coated on silicon dioxide (SiO_2) substrates, aiming to optimize surface-enhanced Raman scattering (SERS) performance. Numerical simulations were performed using COMSOL Multiphysics® to analyze the influence of key parameters—wavelength (532 nm and 780 nm), laser power, and inter-pyramidal gap—on electric field distribution. The study employed the electromagnetic waves, frequency domain (ewfd) interface with the Finite Element Method (FEM) to solve Maxwell's equations, identifying hotspot regions where the electric field intensity is maximized. Results revealed that increasing laser power significantly amplified the electric field due to enhanced electromagnetic energy, while smaller gaps between nanostructures promoted stronger plasmonic coupling, yielding higher electric field intensities at the pyramid tips. Experimental validation using 4-Mercaptobenzoic acid (4-MBA) as a Raman reporter molecule confirmed the simulation findings, with Raman mapping demonstrating greater SERS signal intensity on substrates with narrower inter-pyramidal gaps. The study highlights the critical role of geometric parameters in plasmonic field enhancement and provides design insights for optimizing SERS substrates. Future work will focus on improving fabrication techniques to achieve sub-micron gaps and exploring the substrate's application for environmental biosensing.

Keywords: SERS, plasmonic substrate, COMSOL Multiphysics®, electric field, LSPR, nanostructure simulation.