Evaluating Nanogaps in Ag and Au Nanoparticle Clusters for SERS Applications Using COMSOL Multiphysics®

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Abstract

Silver and gold nanoparticles are widely used in the field of surface enhanced raman spectroscopy (SERS) because of the unique plasmonic properties. Plasmons or surface plasmon resonance result from the wavelength dependent dielectric properties of noble metals like Ag, Au, Pt etc., which give rise to enhanced near-electric field which is the primary reason for enhancement of Raman signal in SERS[1, 2]. Furthermore, the major contribution for the enhancement in SERS comes from the hotspots generated in the nanogaps of the nanoparticle assemblies of the prepared substrates. Therefore, the inter-particle distance and particle size is a significant factor in estimating the enhancement factor in SERS. In this study, we aim to estimate and predict the size and nanogaps to optimize the SERS application using COMSOL Multiphysics®. Additionally we also corroborate the theoretical results with SERS experiments by building an ultrathin polymer shell around the nanoparticles using layer-by-layer method, in which the polymer shell acts as a separating inter-particle spacer layer. This will help identify the optimal arrangement of nano assemblies and the required excitation wavelength depending on the application.

The near-field enhancement studies are performed by finite element analysis using wave optics physics in COMSOL Multiphysics®. A plane wave polarized in the Z-axis direction and propagating along the X-axis direction was used for solving the scattered field of Maxwell's wave equations in a wavelength domain study. The incident excitation wavelength of the monochromatic plane wave is the same as the incident laser wavelength of Raman microscope used in the experiments. In other studies, appropriate surface plasmon resonance wavelength is chosen corresponding to the nanoparticle system so that the maximal field enhancement is simulated after excitation at the SPR maximum.

This study exhibits how the FEM and field simulations using COMSOL Multiphysics® can act as a vital mechanistic tool to understand the plasmonic properties of silver and gold nanostructures; and visualize their near-field enhancement, which helps in more straightforward nano-engineering of substrates in SERS.

References:

1. Stiles, P. L. & Van Duyne, R. P. et al. Surface-Enhanced Raman Spectroscopy. Annual. Rev. Anal. Chem.1, 601-26 (2008).
2. Schlucker, S. Surface-Enhaced Raman Spectroscopy. Angew. Che. Int. Ed. 53, 4756-95 (2014).

Figures used in the abstract

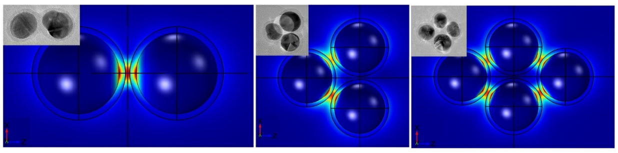

Figure 1: Dimer, trimer and tetramers of Ag nanoparticles with polymer spacer layer exhibiting the hot spots generated because of surface plasmon resonance.