Shell-Isolated Nanoparticle-Enhanced Raman Spectroscopy: Insight From Simulations with COMSOL Multiphysics® Software

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Abstract

Surface-enhanced Raman spectroscopy (SERS) has been developed as a versatile tool for trace-molecule detection and biomolecular analysis by coupled gold or silver nanostructures in the past two decades. However, SERS suffers from a long-term limitation of application for surface analysis of general materials. That is because the SERS hotspots in inter-particle nanogap generated from coupled nanostructures are spatially tiny (~ 25 nm2), and the typical materials such as silicon wafer and blades in motors could not be squeezed into hotspots in the inter-particle nanogap. And the SERS hotspots were not specially designed on the surface of probe materials. Furthermore, several interfered Raman signals typically could not be ruled out if we employ the contact-mode SERS based on bare Au or Ag nanoparticles. We develop the shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) by designing nanoparticles with plasmonic gold core with ultrathin silicon shell as a SERS enhancer. When the core-shell nanoparticles are spread on a material surface, Raman signals of the species on the surfaces of probe materials could be significantly enhanced.
With the help of Wave Optics Module of COMSOL Multiphysics® software, we successfully modelled the enhancement factor of SHINERS on metal and dielectric substrate surfaces. In the simulation, we employed the analytic background field instead of using two-step calculations. The simulation made with COMSOL® software further help us to design new generation shell-isolated nanoparticles with much high SERS activity.