A Reliable Approach to Estimate Surface-enhanced Raman Scattering Intensity of Metal Nanostructures

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Abstract

Surface-enhanced Raman scattering (SERS) is a fingerprint spectroscopy whose sensitivity is down to single molecule level. The mechanism of SERS is mainly contributed to huge enhancement of local electric field, which originated from surface plasmon resonance of metal nanostructures. It is very important to exactly calculate the local enhancement in the electric field strength for right estimation of the SERS enhancement factor.
We use Wave Optics Module and the Electromagnetic Waves, Frequency Domain functionality in COMSOL Multiphysics® software to conduct the simulation. The model of a gold nanosphere is established to solve the scattered field. The background electric field is determined by analytical solution without the gold nanosphere. The molecule is assumed to be uniformly adsorbed on the surface of gold nanosphere. The average enhancement in the fourth power of electric field (|E|4) at the surface of the nanosphere is employed to estimate the SERS enhancement factor. In other word, we set a surface integration to integrate the surface normE of the gold nanosphere. However, this result might be incorrect because of the discontinuity of the electric field at the surface.
Here, we provide two approaches to get reliable results. The first one is to draw a parameterized surface very close (such as 0.1nm outside) to the surface to the nanosphere, and to calculate the average |E|4 on the parameterized surface. The second one is to calculate the average |E|4 on the outer surface of the gold sphere. As shown in the Fig. 1, the proposed two approaches (red and blue dotted lines) are more reliable than the direct integration method (black dotted line) in correctly estimating the SERS enhancement.

Reference

1. S. Y. Ding, et. al. Nanostructure-based plasmon-enhanced Raman spectroscopy for surface analysis of materials. Nature Reviews Materials, 1, 16021 (2016).

Figures used in the abstract

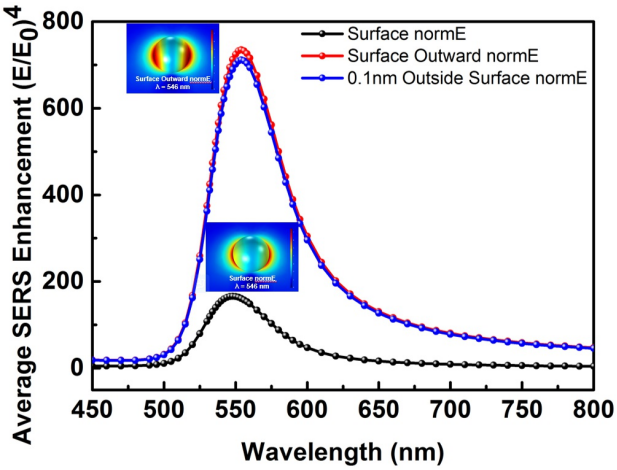

Figure 1: Figure 1 Frequency-dependent spectra of the estimated average SERS enhancement by three different approaches.