Increased Efficiency in Tip-Enhanced Raman Spectroscopy

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Tip-enhanced Raman spectroscopy (TERS) is a powerful tool for detecting chemical properties in nanoscale with extremely high resolutions. For example, TERS may be used in cancer research to find the distribution of certain structures and molecules in malignant cells which can provide key insights into future treatments. However, greater enhancements and sensitivities are needed when studying structures at the scale of single molecules. This study analyzed theoretical simulations of TERS, varying the tip and substrate materials using gold, silver, palladium, platinum, and tungsten, and adding additional nanoparticles with varying radius of 5-15 nm and varying distances from the tip vertex of 15-30 nm to compare changes in enhancement and size of the localized near-field, which is a crucial factor in increasing sensitivity. Plasmon resonances of systems were found using Fourier analysis and implemented for optimal results. A finite-difference time-domain (FDTD) method with subgridding was used to provide accurate enhancement values and analysis of the size of the near-fields. Maximum enhancement of the tip-substrate gap was found with a silver tip and substrate, the enhancement being 3.49 times that of a gold tip and substrate. A silver tip and substrate with nanoparticles of 5 nm radius 20 nm away from the tip vertex resulted in the most localized near-field with the full width at half maximum of the enhancement distribution being 2.96 nm. Although the most localized near-fields did not necessarily produce the greatest enhancement, the unprecedented study of greatly localized near-fields within FDTD can provide better TERS resolution and opens up new frontiers and greater capabilities for TERS.

Awards Won: