## High-Resolution Near-Field Nanoscopy Simulation Platform for Nanomaterial Characterizations

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Scattering-type scanning near-field optical microscopy (s-SNOM) is a state-of-the-art optical technique to probe the dielectric properties of materials in the nano-scale. Only requiring minimal sample preparation, s-SNOM provides 2D scans and "fingerprint" spectra of diverse materials such as photonic devices, biological molecules for cancer cell and virus imaging, and chemicals for trace explosive detection. Despite advancements in s-SNOM experimental techniques, the predictive power of current s-SNOM analytical approximation models is limited by s-SNOM signal dependence on probing tip shape. In addition, previous numerical s-SNOM simulation did not incorporate harmonic demodulation, an experimental signal extraction procedure. To address current limitations in s-SNOM simulations, a demodulation-based tip-modeling (DBTM) simulation was developed in this work, incorporating both a cone-shaped probing tip and harmonic demodulation. The accuracy of the DBTM simulation was confirmed by predicting near-field spectra and spatial signal contrast in SiO2 (weakly resonant), Al2O3 (strongly resonant), and nanodisk structures at the technologically important infrared spectral range. In SiO2 simulation, 55° - 65° was identified as the optimal angle of incidence for maximum near-field signal. The DBTM simulation predicted phonon resonance frequencies of Al2O3 more accurately than the conventional point dipole model. In the nanodisk simulations, near-field contrast in the spatial domain between Al2O3 and Au was demonstrated, and an unprecedented simulated s-SNOM spatial resolution of under 30 nm was achieved. The accuracy of DBTM simulations enables low-cost time-efficient development of novel nanomaterials and future systematic optimization of s-SNOM resolution and capabilities.

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