THE EFFECT OF SURFACE ROUGHNESS ON THE EXTINCTION SPECTRA AND ELECTROMAGNETIC FIELDS AROUND GOLD NANOPARTICLES

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INTRODUCTION

When molecules are absorbed on metallic nanoparticles, the Raman signal can be enhanced by several orders of magnitude, a process known as surface-enhanced Raman spectroscopy (SERS). SERS has been broadly applied, including biosensing and solar cell applications, and its enhancement mechanisms have been extensively studied by experiments and theories for the past 30 years. (1) Among the different enhancement mechanisms, the enhancement in electromagnetic field due to plasmon excitation in the metal nanoparticle is generally considered to play the dominant role. (2) The plasmonic resonance frequency can be tuned by the shape and the size of nanoparticles. (3) And the topography of the particles's surface also has significant effect to the intensity of SERS, which is more important in surface-enhanced single molecule spectroscopy. (4) Here, we will study the effect of surface roughness on the extinction spectra of gold nanoparticles and electromagnetic field around them.

COMPUTATIONAL METHODS

The gold disk dimers are studied by Discrete Dipole Approximation (DDA). (5) The diameter and the average thickness of gold disks are 360 nm and 120 nm, respectively. The gap between them is 32 nm. The rough surface has the vertical RMS of 8 nm and the horizontal correlation length of 18 nm, which is roughened by random deposit method. (6)

RESULTS

Extinction spectra are important to identifying plasmon resonance wavelengths. In Figure 1, the extinction spectra of gold dimers are plotted. The black, red and green curves are from experimental measurements, DDA calculation for the dimer with rough inner surfaces and DDA calculations for the dimer with smooth surfaces, respectively. They all agree with each other. The slight discrepancy between black curve and red curve may due to the fact that the gap of gold dimer in experimental measurements is 30±4 nm instead of 32 nm. The little discrepancy between red curve and green curve is due to the rough surfaces.

For gold dimers, plasmon resonance can be excited effectively only when the incident light is polarized along the symmetry axis, so only this polarization is considered and the incident wavelength is 633 nm. In Figure 2, the contours of $|E|^2$ are plotted for the dimer with smooth inner surfaces. There is a huge hot spot in the center of disk-disk gap and the filed around corners get significant enhanced too. The similar contour is plotted in Figure 3 for the dimer with rough inner surfaces. The hot spot in the center of gap is not observed. But there are several new hot spots around the sharp edges of inner surfaces. At the same time, the hot spots around corners are weakened.

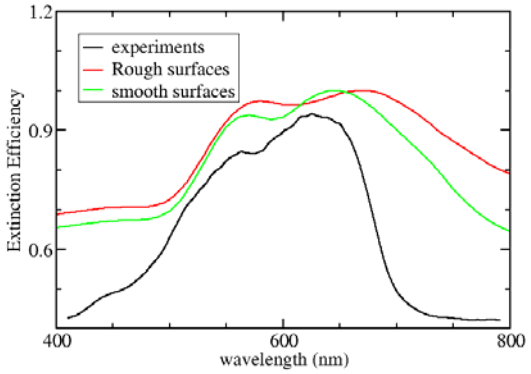

Figure 1: extinction spectra of gold dimers

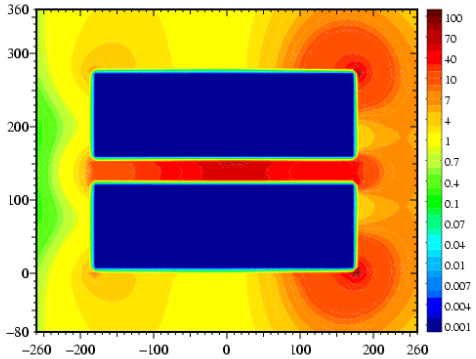

Figure 2: contour plot of $|E|^2$ with smooth surfaces

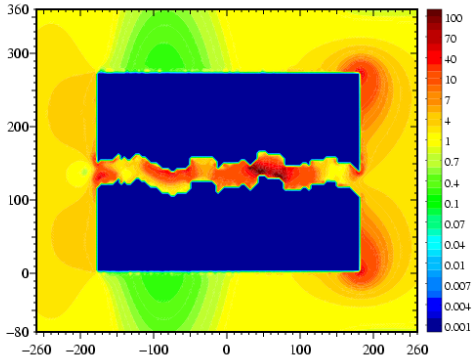

Figure 3: contour plot of $|E|^2$ with rough surfaces

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