Geometry and mesh for PSTD calculation

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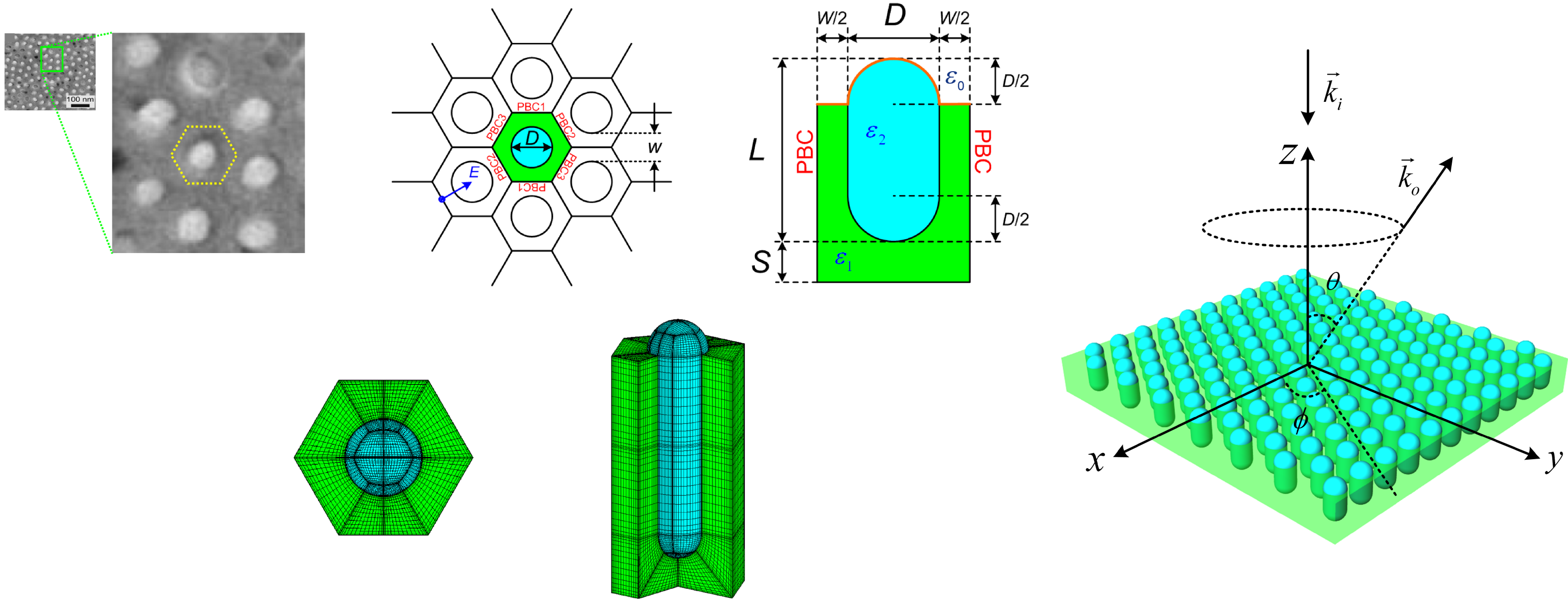

- The Ag nanoparticle array can be considered Ag nanorods arranged in hexagonal pattern with an inter-nanorod gap (*W*). The rod diameter (*D*) is 25 nm and the rod length (*L*) is 100 nm.
- A series of curved hexahedral sub-domains and mesh sampling points therein are created.
- A plane EM wave impinges on the array vertically and the scattered radiation is collected around the cone at q = 45°.
- After the field on the top surface was obtained, the scattered radiation in far field was then calculated based on field equivalence principle.

B.-Y. Lin et al., Opt. Express 17, 14211 (2009).

Calculated scattering spectra

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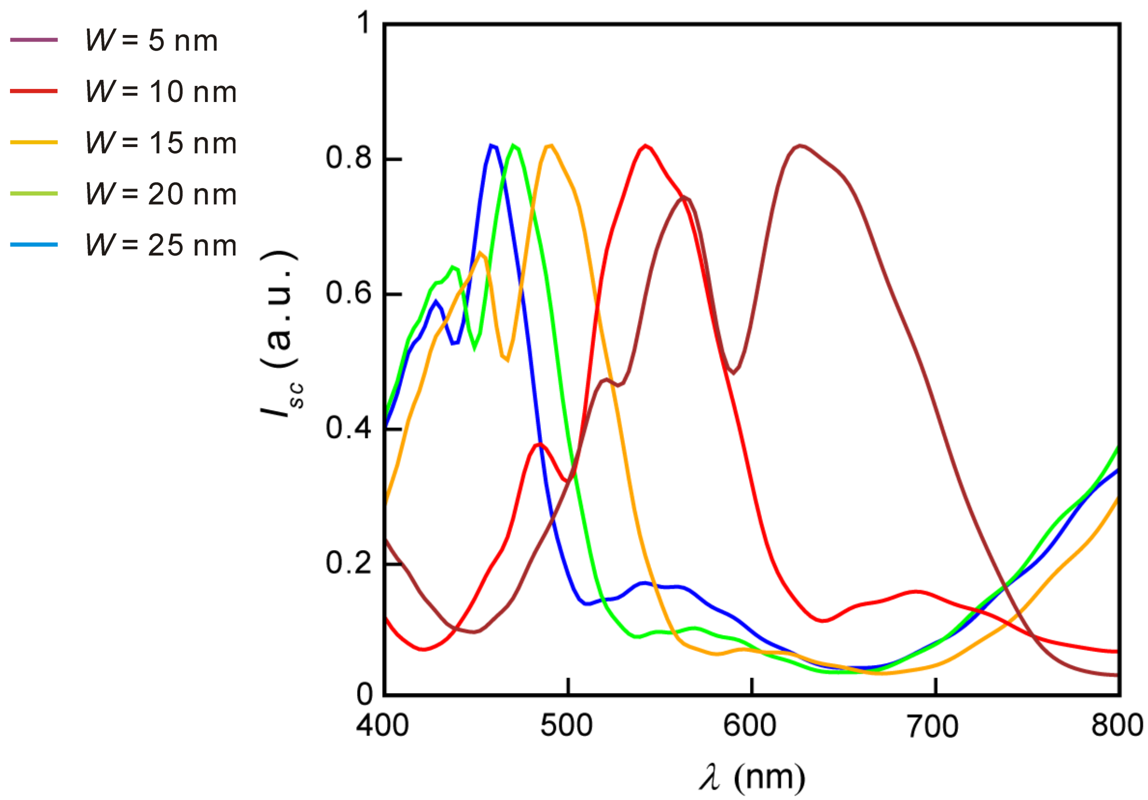

- The calculated far-field spectra follow the experimental data qualitatively: The resonance wavelength increases and the width is broadened as the interparticle gap decreases.

B.-Y. Lin et al., Opt. Express 17, 14211 (2009).

Far-field scattering contributions

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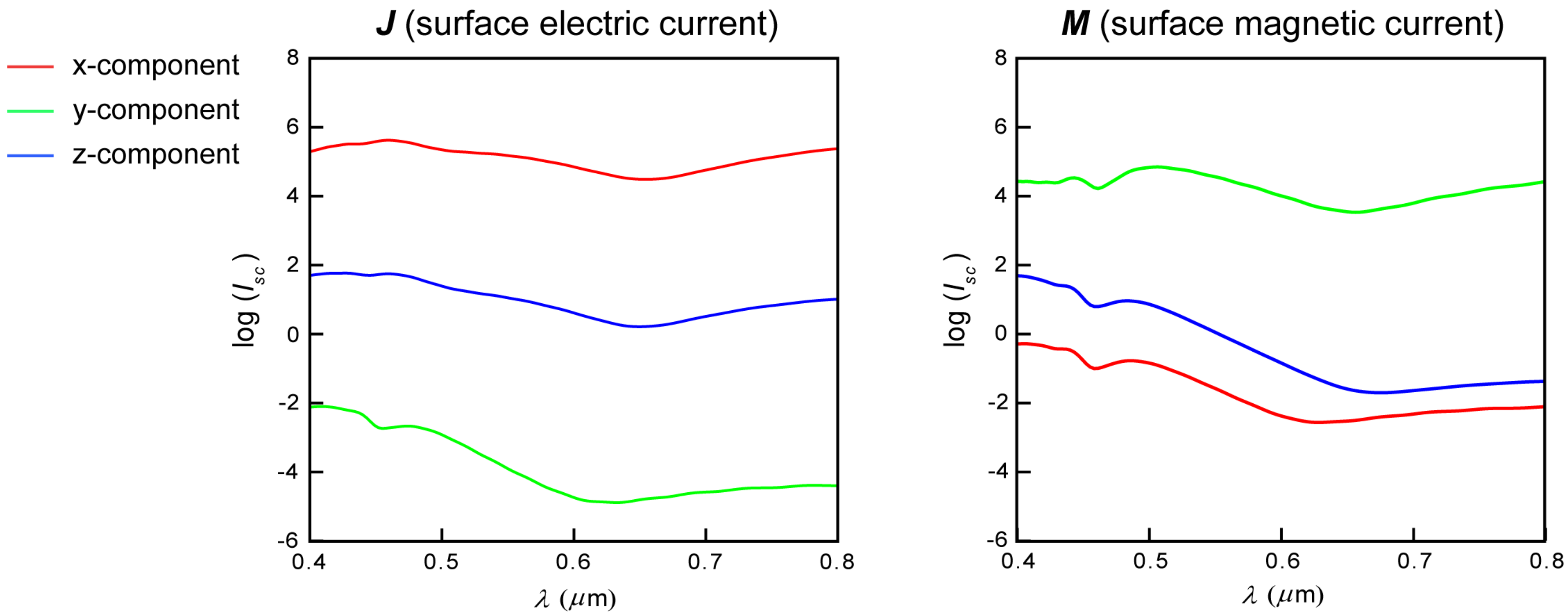

- For all the different interparticle gaps, the far-field scattering is dominated by surface electric current density (***J***) which is generated by surface magnetic field, according to field equivalence principle.
- In contrast, surface magnetic current density (***M***), generated by surface electric field, plays a minor role in far-field scattering.

B.-Y. Lin et al., Opt. Express 17, 14211 (2009); S. R. Rengarajan and Y. Rahmat-Samii, IEEE Antennas Propagat. Mag. 42, 122 (2000).

Surface field distribution

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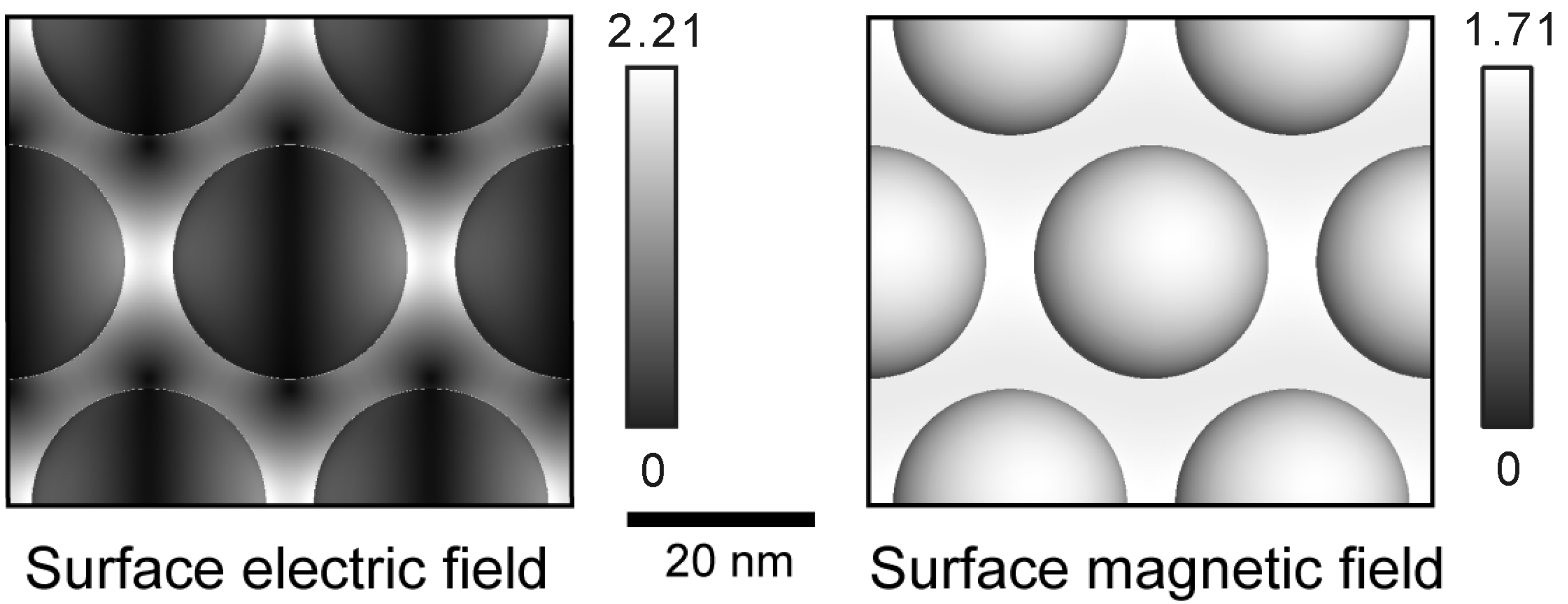

- The surface electric field is localized at the gap region between adjacent Ag nanoparticles.
- The surface magnetic field is delocalized over the whole surface and produces the corresponding ***J*** that acts as the dominant source of the far-field scattering.
- The so-called “hot spots” created by the localized surface electric field has a minor role in producing far-field scattering.

B.-Y. Lin et al., Opt. Express 17, 14211 (2009).

Cross-section view of electric and magnetic fields

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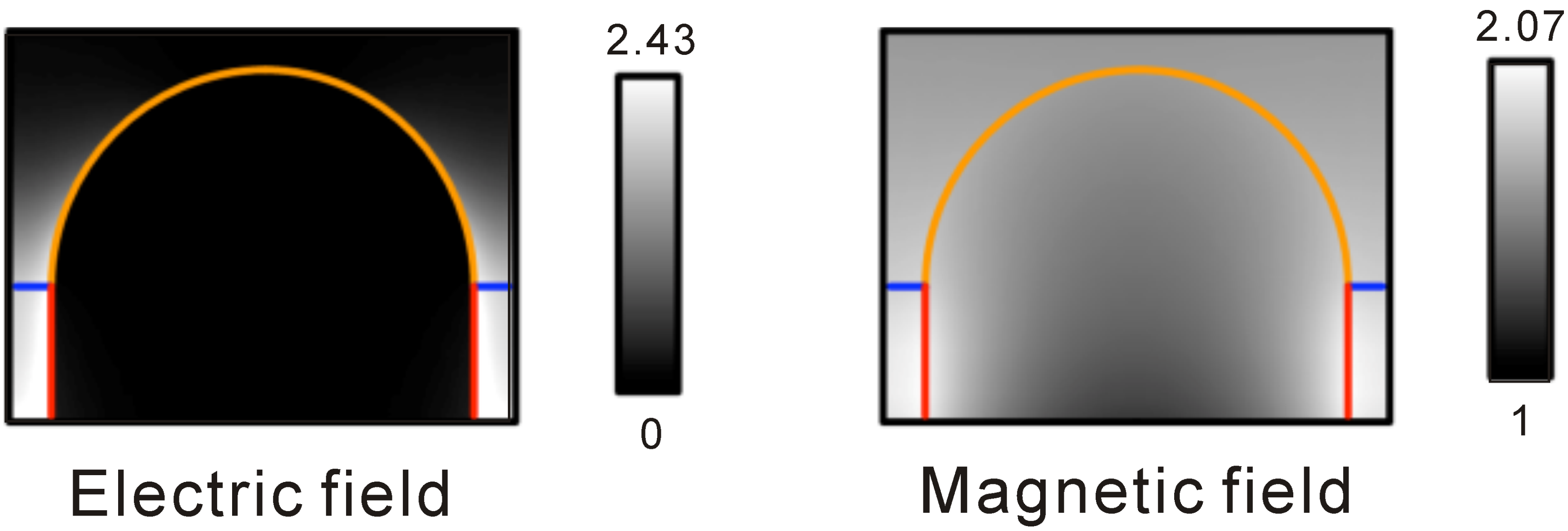

- Electric field resides within the gap and exhibits an evanescent character.
- Magnetic field delocalizes over the surface and shows mainly a propagating character.
- In surface-enhanced Raman scattering, the localized surface electric field interacts with the molecules residing in the gap region, producing a similar electric field distribution at a Raman-shifted wavelength. The resultant concurrent surface magnetic field then makes a major contribution to produce Raman scattering field in far distance.

B.-Y. Lin et al., Opt. Express 17, 14211 (2009).

SERS as a biomedical diagnostic tool

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- Raman spectroscopy, providing molecular vibrational information, can become a powerful and useful method to identify molecular species if its scattering cross section can be enhanced many orders of magnitude.
- Surface-enhanced Raman scattering (SERS) may serve as the solution.
- Most of Raman enhancers have suffered two major drawbacks: low reproducibility and small dynamical range. Therefore, a lot of efforts have been made to control its enhancement mechanisms such that uniform high sensitivity can be achieved.
- One key point is whether it is possible to control precisely the electromagnetic enhancement factor induced by plasmonic resonance.
- Theoretical and experimental studies indicate that the precise control of gaps between nanostructures in the sub-10 nm regime, 'hot junctions', is likely to be critical for the fabrication of SERS-active substrates with uniformly high Raman enhancement factor.

SERS detection of bacterial cell wall

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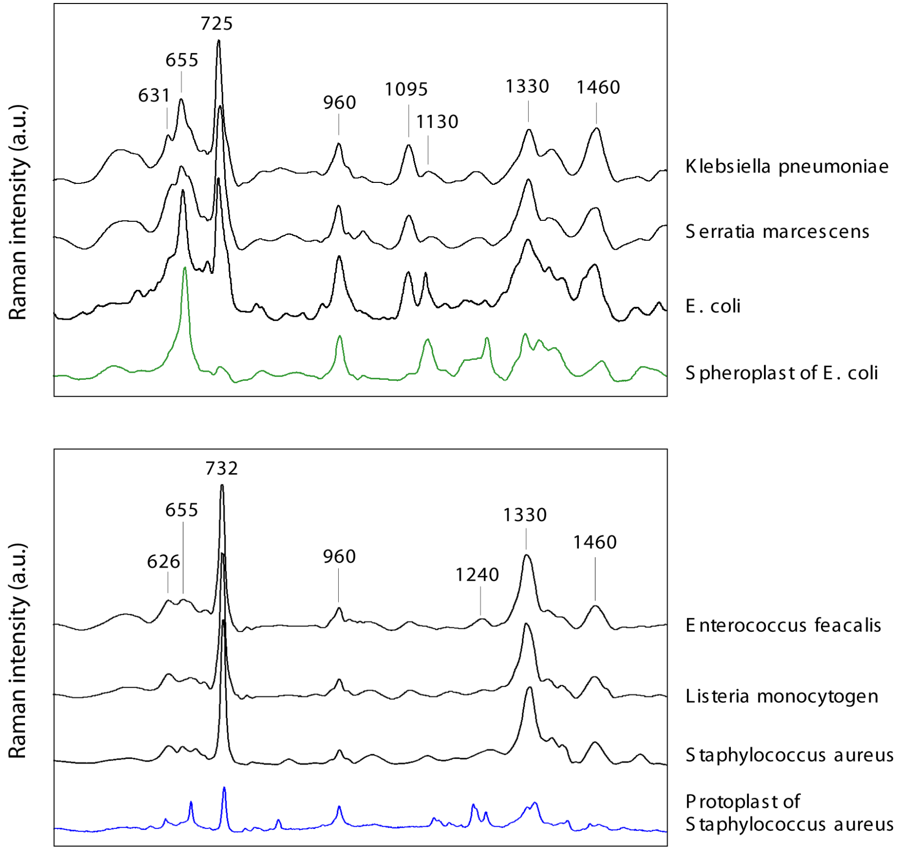

- These substrates are commercially available.

T.-T. Liu et al., PLoS ONE 4, e5470 (2009).

Antibiotic susceptibility testing with SERS

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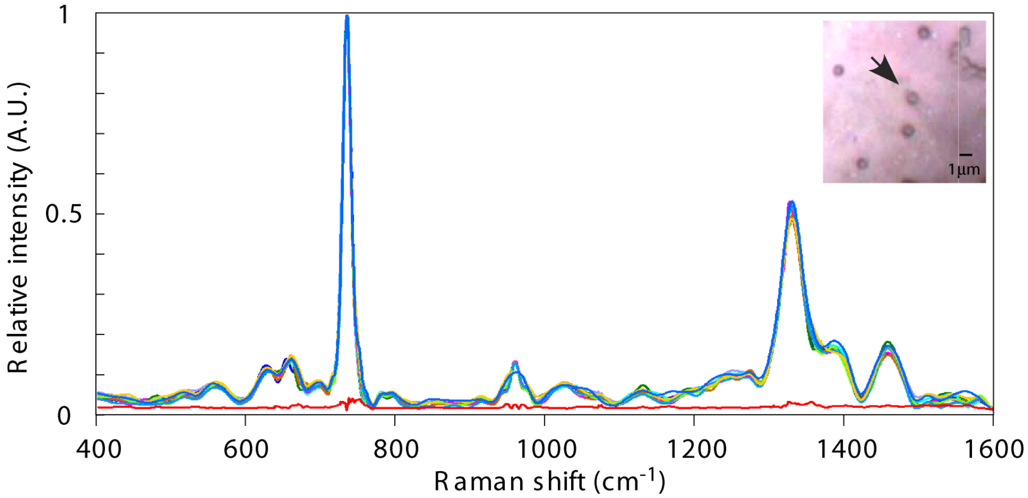
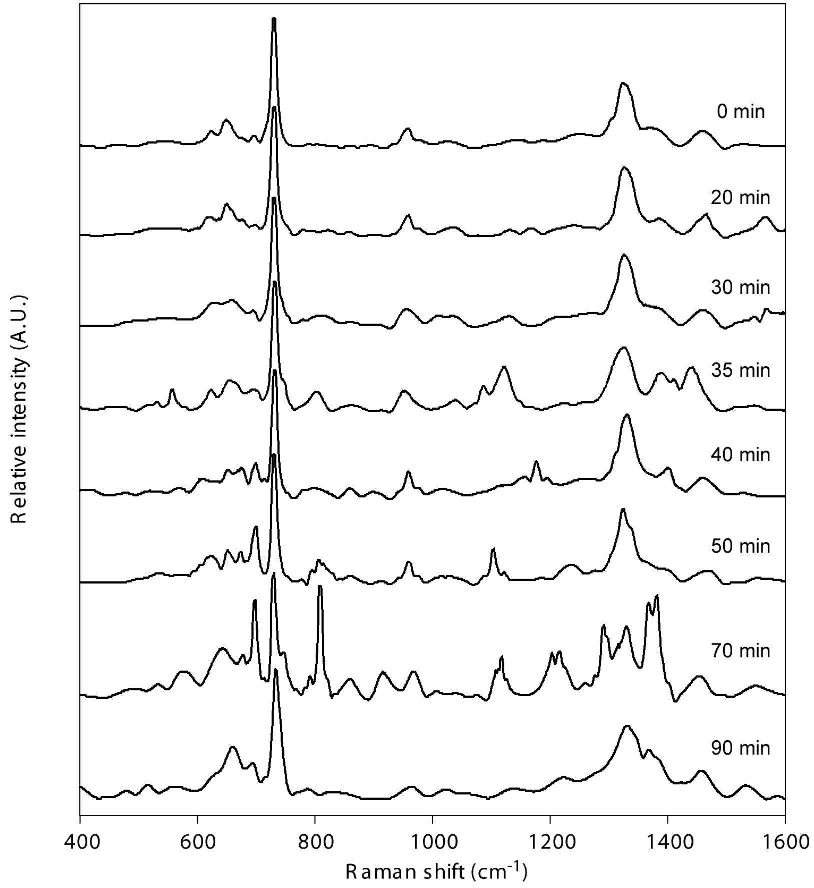
Staphylococcus aureus 13649 treated with vancomycin





- Drastic change in SERS spectra was observed when treated with vancomycin.

T.-T. Liu et al., PLoS ONE 4, e5470 (2009).

Response of *S. Aureus* to different anitibiotics

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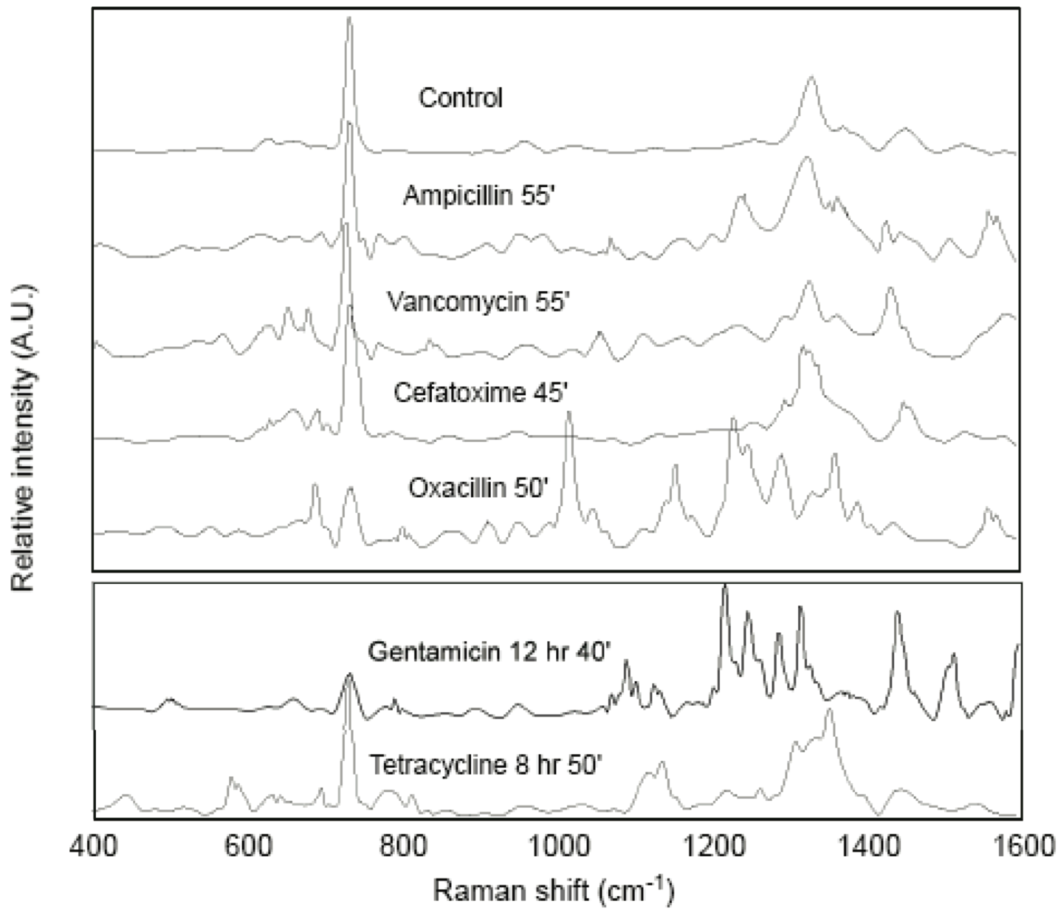

Inhibition of Cell Wall Synthesis (most common mechanism)

Inhibition of Protein Synthesis (second largest class)

- *S. Aureus* responds within 2 hrs to the antibiotics which inhibit cell-wall synthesis, while the response is delayed to longer than 8 hrs. for that which inhibit protein synthesis.

T.-T. Liu et al., PLoS ONE 4, e5470 (2009).

Conclusions

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- Scattering-type SNOM has been demonstrated to serve as a nanoprobe to investigate local optical properties and to probe local field distribution.
- The uniform and highly reproducible SERS-active properties and the wide dynamical range facilitate the use of SERS for chemical and biological sensing applications with high sensitivity.
- The electromagnetic interaction in arrays of Ag nanorods embedded in AAO has been investigated thoroughly by both experimental and theoretical methods.