Dataset for SERS Plasmonic Array: Width, Spacing, and Thin Film Oxide thickness optimization

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Modeling and Simulation   **Photonics**

Background/Relevance

- Previously, Dr. Herzog and his research group have published several works regarding plasmonics in Au nanostructures.
- Other researchers have published computational work that should yield similar results but have gotten discrepancies.

Innovation

- Publish our data and methods in the open-access MDPI Journal DATA to allow other researchers to verify and validate our work.
- Make our data available in a universal format that can be tested with computer modeling software other than COMSOL, such as MATLAB.
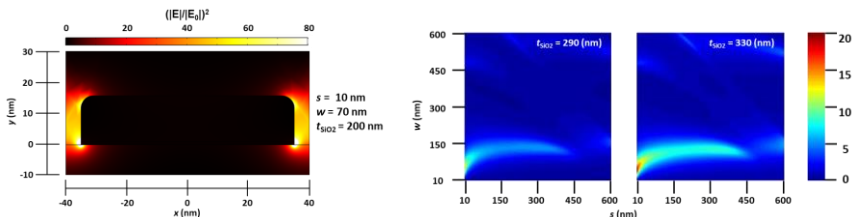
Methods

- Computationally model an array of Au nanowires on an SiO_2 substrate with various parameters.
- Perform with COMSOL, a physics modelling software using finite element method (FEM).
- Vary the widths of the nanowires (w), the spacings between the wires (s), and the depths of the SiO_2 (t_{SiO2}) and analyze plasmonic enhancement for each variation
- Export data into plaintext text files to make accessible to researchers without COMSOL.

- 2D model of array

- 3D render of wire array
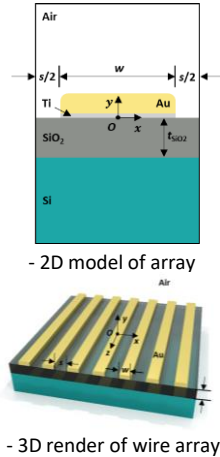
Key Results

- Differing values of s and w at the nanoscale provide varying degrees of plasmonic enhancement.
- There exist parameter combinations that provide strong plasmonic enhancement at values previously unstudied.
- Periodic values of t_{SiO2} provide periodic amounts of plasmonic enhancement, apparently irrelevant to the rest of the structure.

$s = 10$ nm
$w = 70$ nm
$t_{SiO2} = 200$ nm

- Optical enhancement of a specific simulation

- Variations of plasmonic effects between two values of t_{SiO2}

Conclusions

- Stronger than expected plasmonic interference occurs in nanowires spaced greater than 100 nm apart, an area of plasmonics that has not been investigated much.
- This can possibly be utilized for creating substrates for surface-enhanced Raman Spectroscopy (SERS).
- The data can be evaluated in other modelling softwares to allow for accurate validation by fellow computational modelling researchers.