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SERS substrate

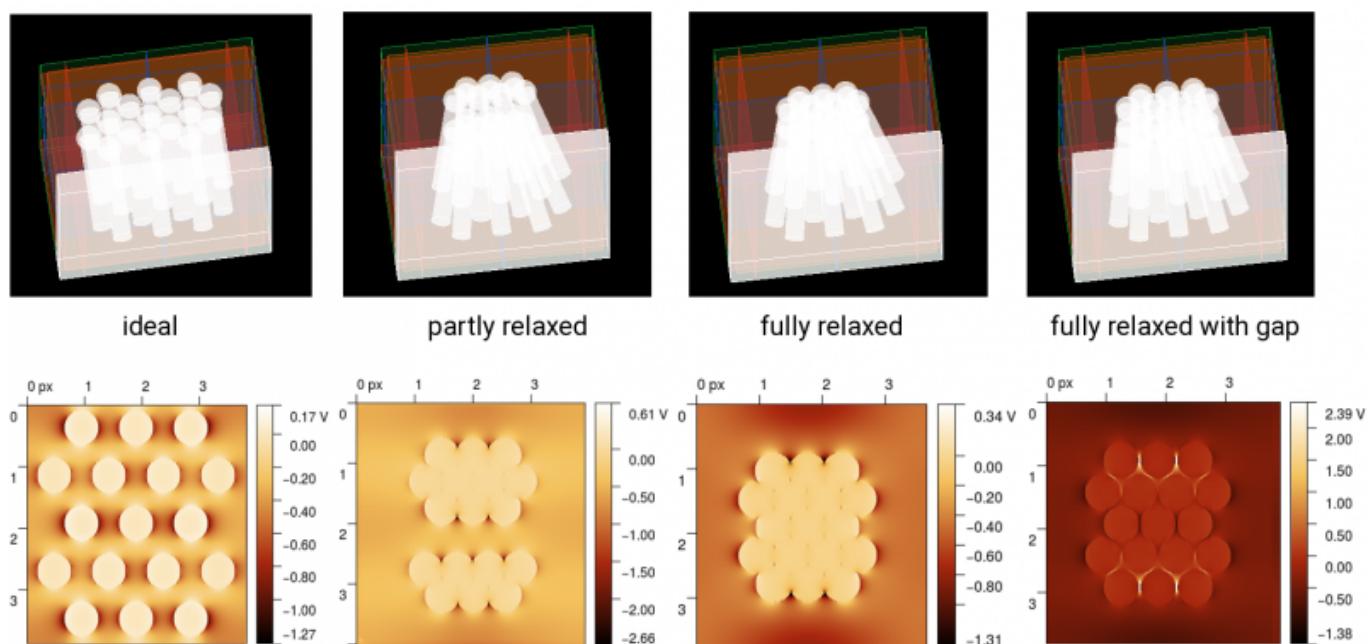
Surface Enhanced Raman Scattering (SERS) is an advanced experimental technique for measurement of Raman scattering signals. Raman scattering itself is a process with very small yield and to measure Raman signals on some individual molecules or thin film materials is very challenging. By placing the investigated material on a special substrate we can increase the signal intensity by several orders of magnitude. The effect is based on local field enhancement which is a plasmonic effect that happens if the sample surface is formed by suitable material and has a suitable geometry.

In the literature there are many suggested surface structures to be used as SERS substrates. Novel materials and geometries are also constantly being developed, focusing on higher yield, cheaper manufacturing and easier use.

Here we show an example of the calculation setup for a SERS substrate on a bit more complex geometry, inspired by work in Ref. 1. This is based on flexible gold coated silicon nanowires. By different manufacturing conditions, the level of self-organization of the top spheres and their geometrical properties can be controlled. Using GSvit we tried to setup models that would potentially include all these parameters.

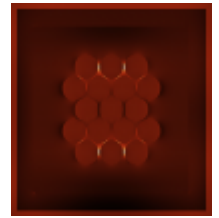
The model was based on a simple script in C that, based on geometrical parameters of the nanowires, their variance and total number, created a material file for GSvit, like shown below. To be able to simulate the partial relaxation of the particles, we have run a simple molecular dynamics like particle relaxation to let the tops of nanowires close together. Mechanical properties of the nanowires were treated only very simply, assuming that the lateral force is proportional to the shift from ideal position.

In the next figure some XSvit screenshots and resulting field distributions from small scale simulations are shown. A sample parameter file (with generated material file) is provided to play with the settings like illumination.



Sample parameter file: [SERS](#).

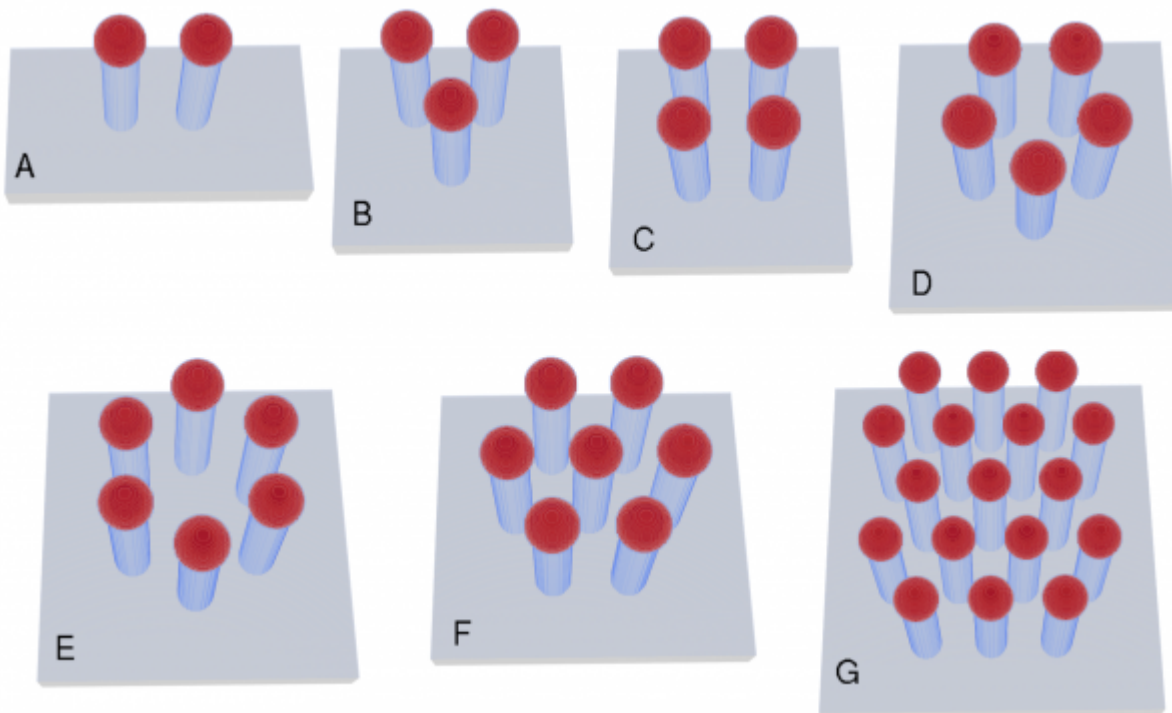
A 340x361x225 computational domain with partly relaxed flexible SERS rods. Periodic boundary conditions are used to simulate an infinite layer. A plane wave with wavelength of 633 nm illuminates the structure from the top, using the layer compatible variant of the total/scattered field source.



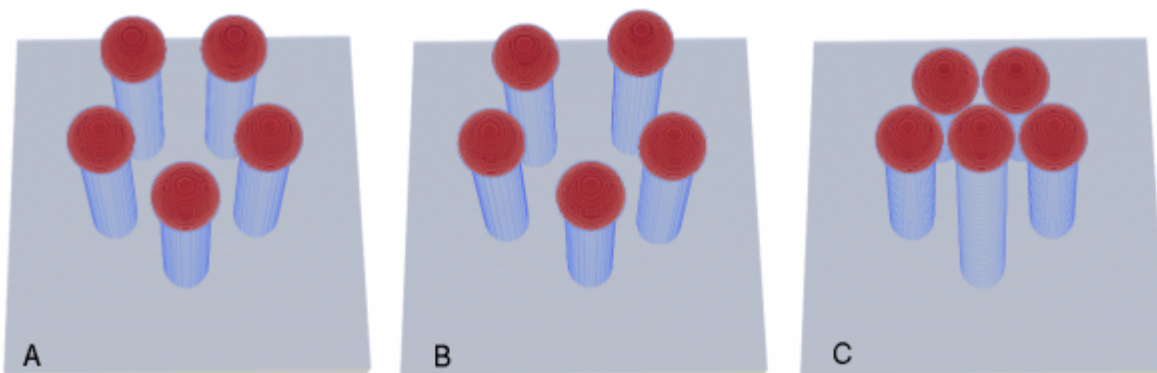
To show how the parameter and material files can be generated, we add here the C program that was used for the calculations:

sersgen2.c

. It allows creating wide range of geometries like shown in the above images. The main types of nanorod placements are (A) linear, (B) triangular, (C) rectangular, (D) pentagonal, (E) circular and (E-F) various amounts of hexagonally packed rods as shown in the following image.



User can control the size of rod components, periodicity and add some imperfections, like imperfection in the rod position and relaxation of the rod, as shown here.



This can be further combined with ability of GSvit of creating surface roughness. In this way dependences of the local field enhancement on some particular parameters can be generated, combining the simple C program, GSvit and some post-processing, e.g. in Gwyddion or using batch processing tools derived from Gwyddion.

Examples: to be added.

Reference

[1] S. A. Kara, A. Keffous, A. Giovannozzi, A. Rossi, E. Cara, L. D'Ortenzi, K. Sparnacci, L. Boarino, N. Gabouze, S. Soukane, (2016). Fabrication of Flexible Silicon Nanowires by Self-assembled Metal Assisted Chemical Etching for Surface Enhanced Raman Spectroscopy. RSC Adv. 6. 10.1039/C6RA20323J.

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