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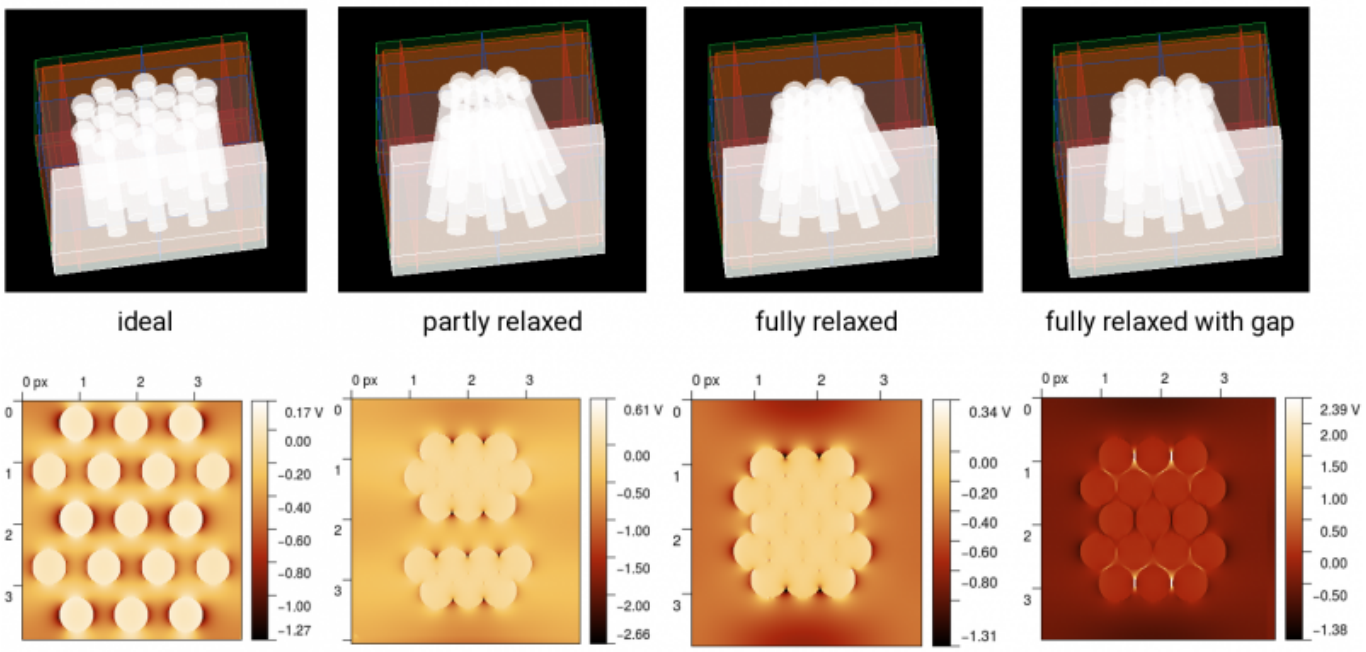
SERS substrate

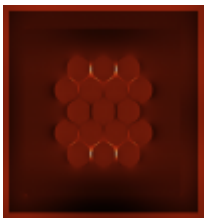
Surface Enhanced Raman Scattering (SERS) is an advanced experimental technique for measurement of Raman scattering signals. Raman scattering itself is a process with very small yield and to measure Raman signals on some individual molecules or thin film materials is very challenging. By placing the investigated 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-organisation of the top spheres and their geometrical properties can be controlled. Using GSvit we tried to setup models that would



Sample parameter file: SERS.
A 300x300x300 computational domain with SERS rods



[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.