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TERS field enhancement

Tip Enhanced Raman Microscopy is, besides SERS another approach how to locally enhance the Raman scattering signal.

There are the few different effects that we can observe when illuminating a nanoscale metallic structure. First of all, we can observe effect of spectral properties of the particular metal from which the structure is formed. Even the simplest possible quantity observed on metals in everyday life - its excellent reflectivity - is material dependent and the different appearance of different metals is its consequence. This can be handled via FDTD easily as there are many different algorithms enabling us to parametrize the spectral dependence of optical properties of metal and use them in the calculation. These algorithms also hide fact that the propagation of light through metal described only by its complex permittivity can't be handled easily via conventional grid spacing and time steps. An example of calculated metal reflectivity via FDTD for different metals and algorithms is shown in section Media.

The second remarkeable effects is the antenna effect. When we prepare a structure with size that is comparable to the wavelength of the illuminating light, we form an antenna similarily like e.g. in radio communications. This leads to significant local enhancement of the electromagnetic field around the antenna due to resonance effects. Here we meet the enhancement, which is so important for TERS probes. An example of the antenna effect is shown in discussion of Plasmonic nanoantenna.

The apex also size contributes to the enhancement, by the lighting rod effect, based on its curvature. Finally, we want to see a plasmonic field enhancement, a resonance effect if we use probe and sample that match together. This is however happening only in some measurements, as we often measure on materials that have not this ideal properties.

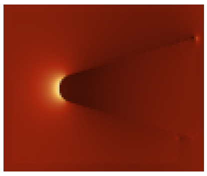
If all these results are combined, we can get many orders of magnitude field enhancements. Very often, however, this is fulfilled only partly and some practical issues related to probes manufacturing and handling also oppose to get an ideal result in many cases.

There are many different results in the literature related to TERS probes. Most typically, the probe is simulated for a single wavelength, using a truncated probe apex and plane wave illumination. This is an easy way how to demonstrate the local field enhancement. However, there are few potential problems:

Even for truncated probe, some antenna effect can be expected (ideally infinitely extending probe is hard to be simulated). Truncated probe is still far from reality as in real experiments, the probe is large, much larger than what can be simulated unless we make the model consisting of really large voxels, losing some spatial resolution (there is a tradeoff between the detailness of model and its size). Staircasing effect can create some extra errors, namely for coarse models.

Nevertheless, we can simulate all the typical effects observed at TERS probes. We focused on aluminium coated silicon probes and first wanted to separate different competing effects, as follows The smaller the tip radius is the bigger is the enhancement. The bigger is the thickness of aluminium layer, the bigger is the enhancement in our spectral region of interest

A series of numerical experiments was done to see these effects separately and combined. First, probes from solid aluminium were simulated, having different radii. Second, probes with the same total radius were simulated, having different thickness of the aluminium layer (so the silicon core radius) was changing appropriately. Finally, the most realistic case which are probes with silicon core of some radius with thin film of varying thickness on top was simulated. The simulations were peformed for different wavelengths and also for different materials of the core.



Sample parameter file: TERS.
A 300x300x300 computational domain with TERS tip
