NanoPhotonics

COMSOL CONFERENCE 2019 BOSTON

Gold-Coated Fumed Silica Monolayer for Efficient Large-Scale SERS Substrates with High Density Nanogaps

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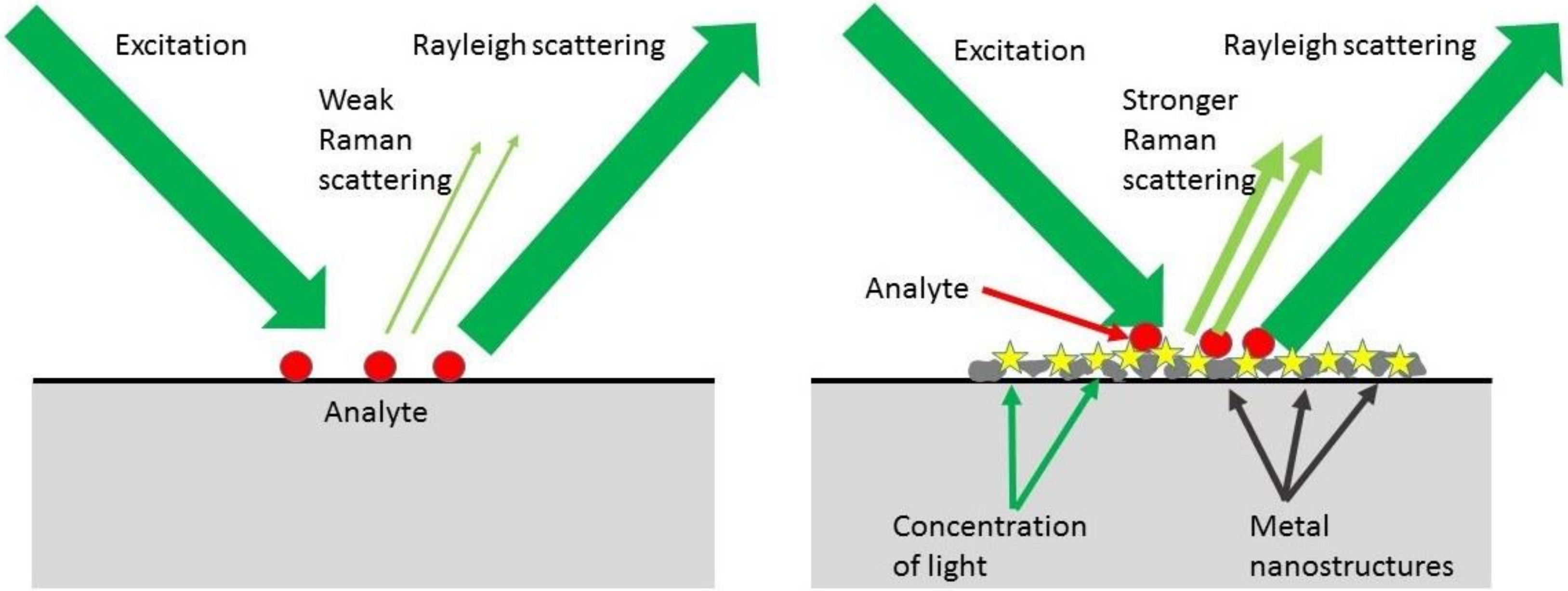
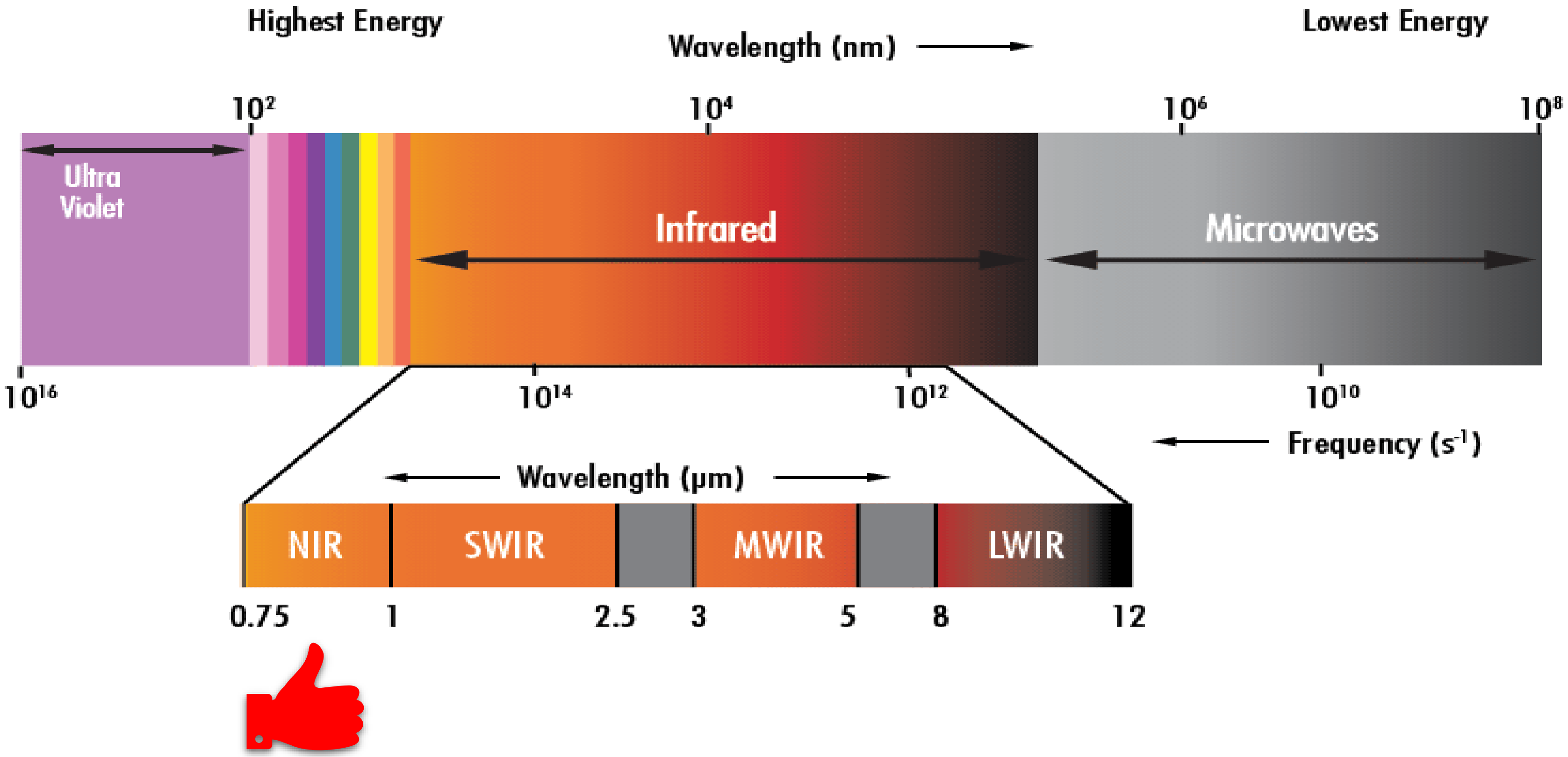
Surface enhance Raman spectroscopy



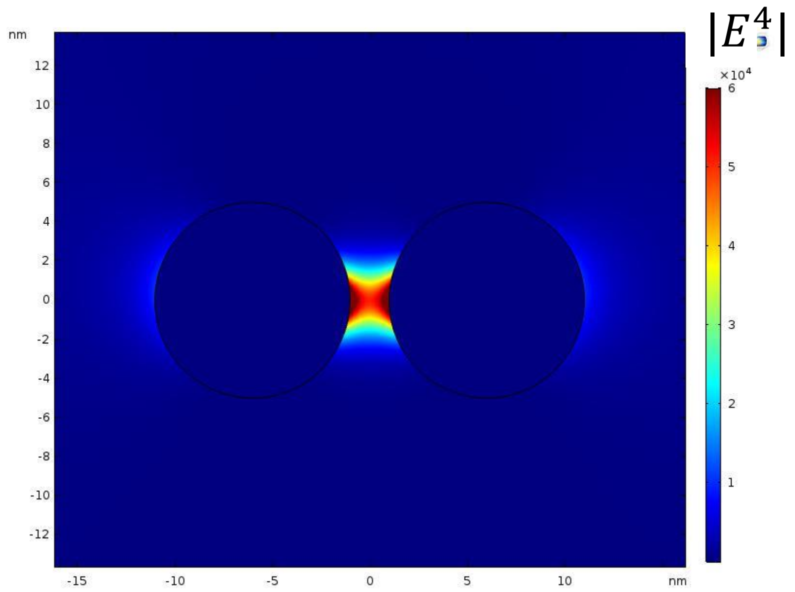
China,(Jan,2019)Global and China Surface Enhanced Raman Spectroscopy (SERS) Market Research by Company, Type & Application 2013-2025,retrive from https://marketandresearch.biz

Near-Infrared

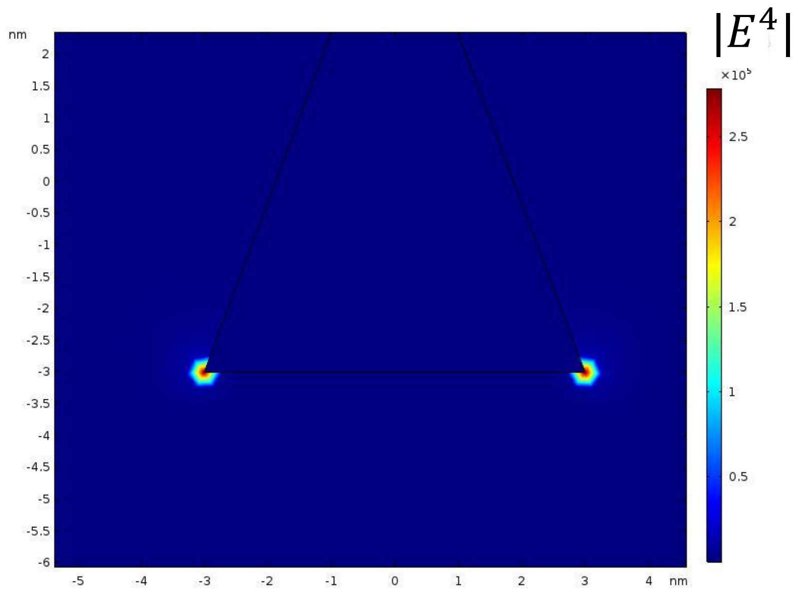


Edmund Optics Inc., What is SWIR?
Retrieved from https://www.edmundoptics.com

The importance of nanogaps

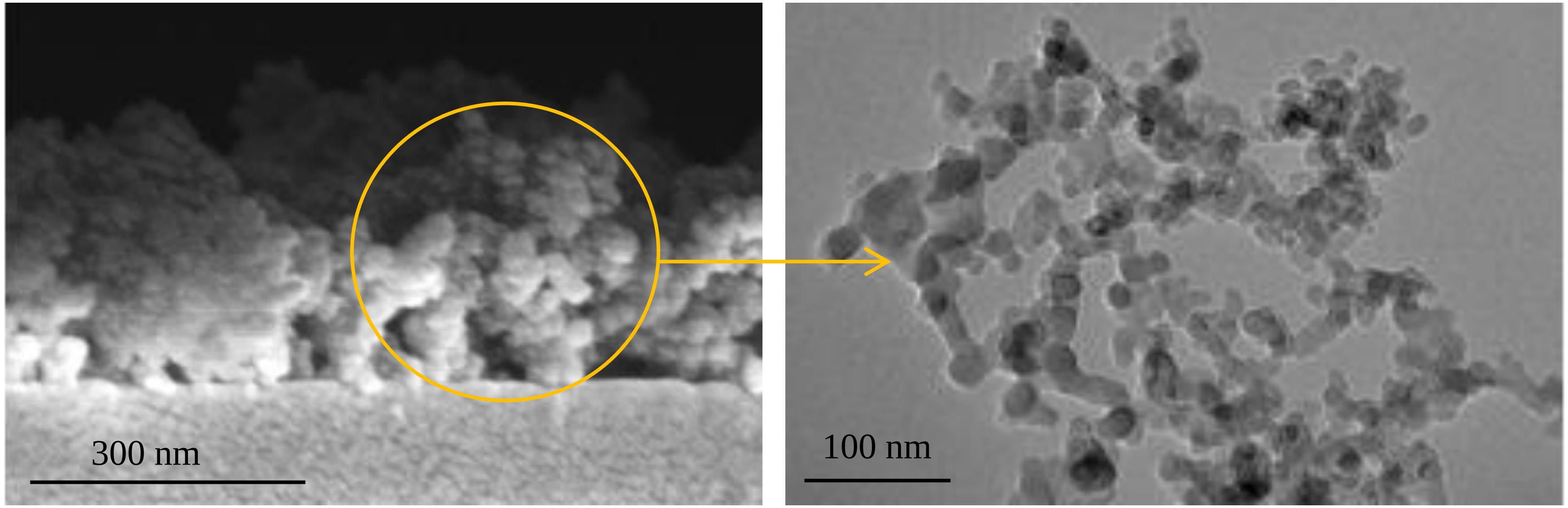


nanogap



nanotips

The importance of fumed silica



Fumed silica becomes SERS template for gold deposition

Objective

- To investigate LSPR properties of SERS substrate, formed by highly porous silica-gold core-shell network structures

- study the resulting plasmonic resonance behaviors, as well as the electric field enhancement factor and absorptance.

- Effect of geometric parameters are including silica particle size, gold thickness and particle density

Maxell’s wave equation

Solve for E

$$\nabla \times \mu_r^{-1}(\nabla \times \boldsymbol{E}) - k_0^2\left(\epsilon_r - \frac{j\sigma}{\omega\epsilon_0}\right)\boldsymbol{E} = 0,$$

σ : *electrical conductivity*
μ_r : relative permeability
ϵ_r : relative permittivity

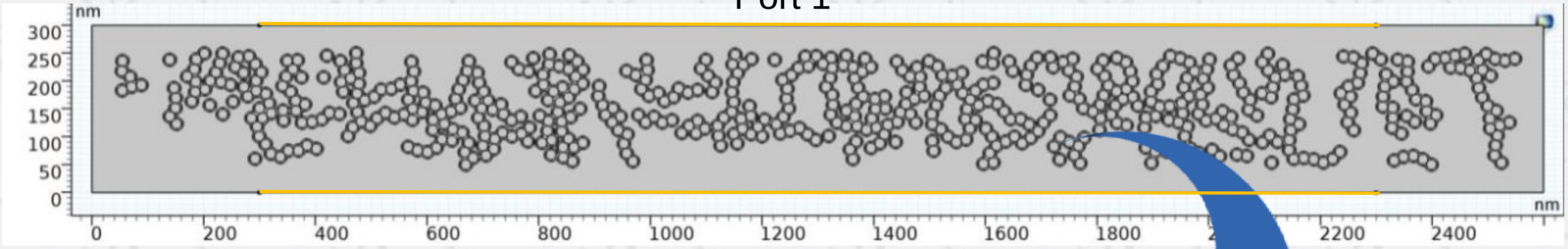
$$n = \sqrt{\epsilon_r\mu_r}; \mu_r \approx 1$$

$$\tilde{\epsilon}_r = \epsilon_r - \frac{j\sigma}{\omega\epsilon_0}$$

$$\boldsymbol{E}(x,y,z) = \widetilde{\boldsymbol{E}}(x,y)e^{-jk_z z}$$

COMSOL MULTIPHYSICS

Port 1

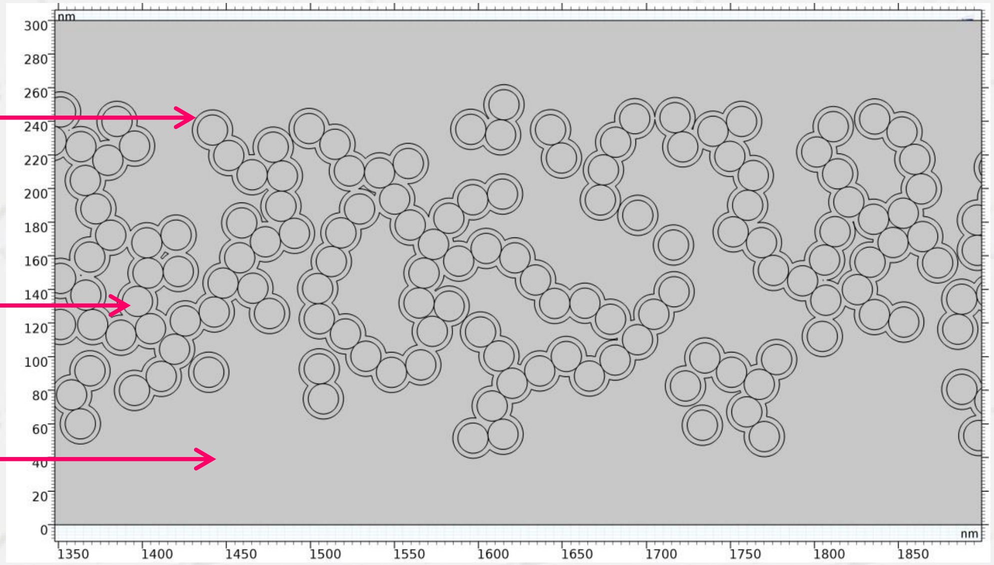


Port 2

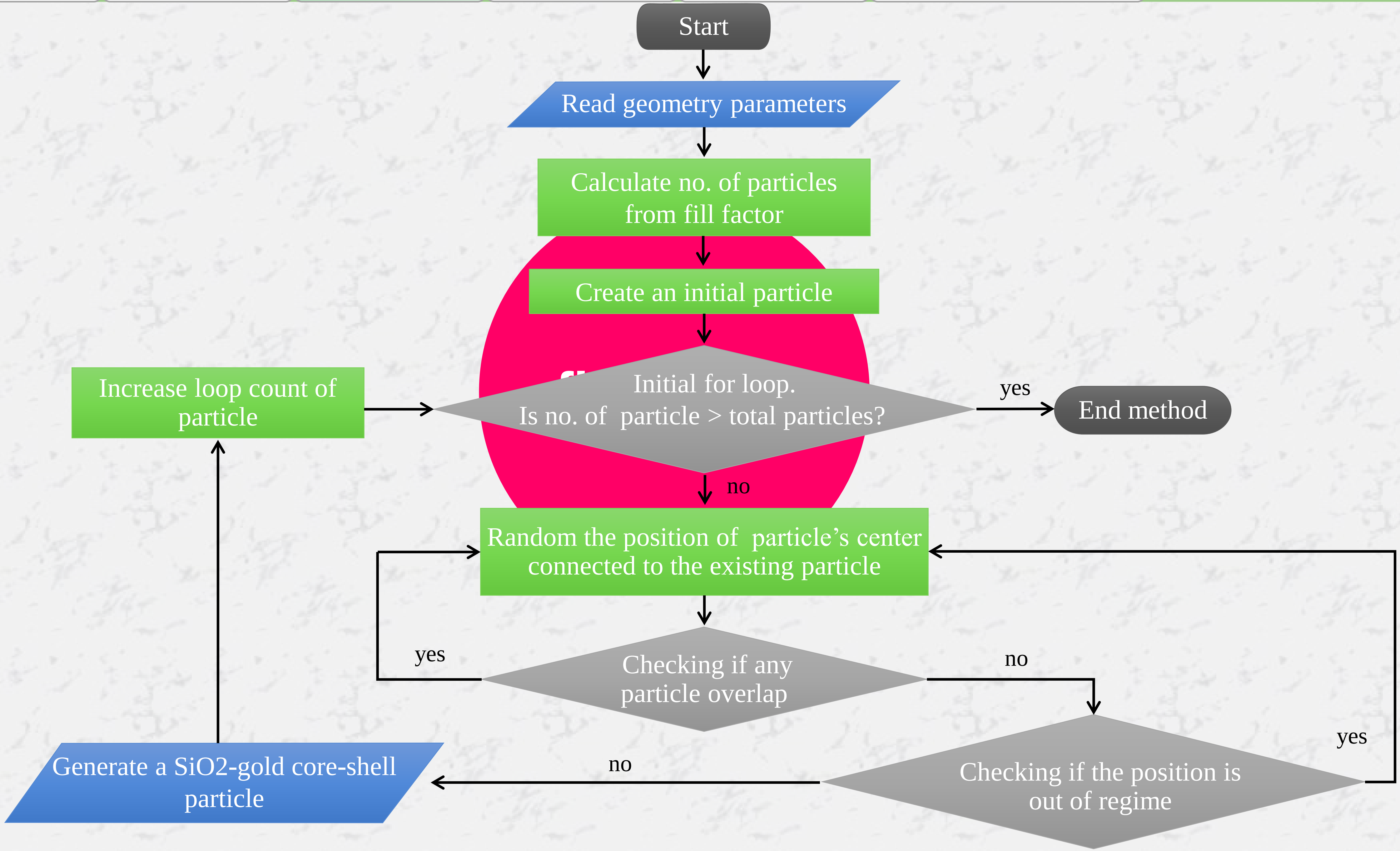
Gold-coated

silica

air



The geometry created by using code in model methods.


Start
Read geometry parameters
Calculate no. of particles from fill factor
Create an initial particle
Initial for loop.
Is no. of particle > total particles?
yes
End method
no
Increase loop count of particle
Random the position of particle's center connected to the existing particle
Checking if any particle overlap
yes
no
Checking if the position is out of regime
yes
no
Generate a SiO2-gold core-shell particle

Choose the module

1.Optics

2.Wave optics

3.Emw, frequency domain

$$\nabla \times \mu_r^{-1}(\nabla \times \boldsymbol{E}) - k_0^2\left(\epsilon_r - \frac{j\sigma}{\omega\epsilon_0}\right)\boldsymbol{E} = 0$$

Define parameters

Parameters	Expression	Description
Lambda	Sweep 300-1500 nm	Incidents lambda of electromagnetic wave
n_{air}	1	Refractive index of air
n_{silica}	Equation	Refractive index of silica
n_{gold}	Build-in parameter	Refractive index of gold
P_{inc}	2.6544E-9 W	Incidents power

Refractive index of silica

$$n_2 - 1 = \frac{0.6961663\lambda^2}{\lambda^2 - 0.0684043^2} + \frac{0.4079426\lambda^2}{\lambda^2 - 0.1162414^2} + \frac{0.8974794\lambda^2}{\lambda^2 - 9.896161^2}$$

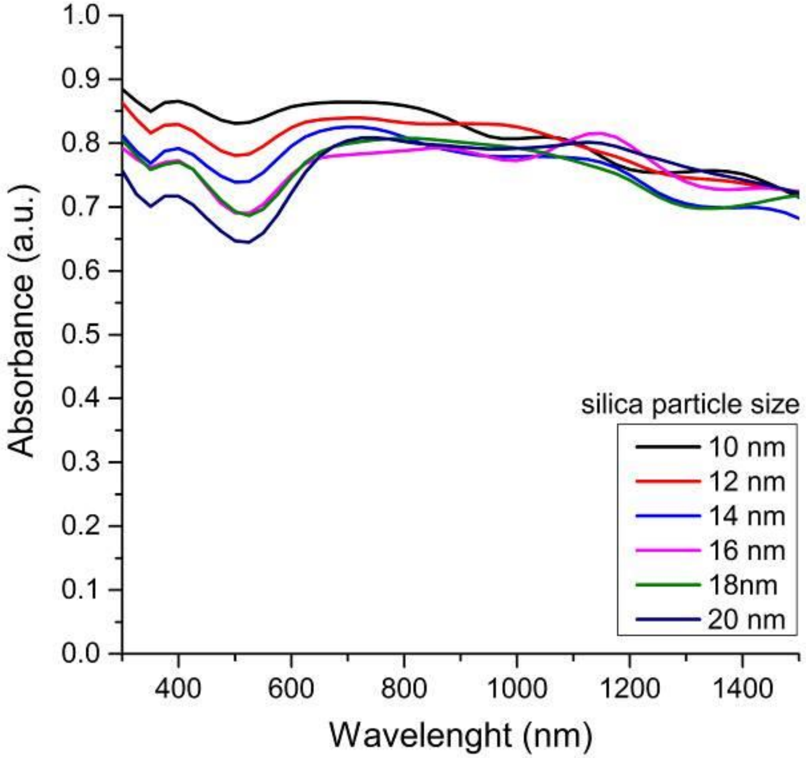
C. Z. Tan. Determination of refractive index of silica glass for infrared wavelengths by IR spectroscopy, *J. Non-Cryst. Solids* **223**, 158-163 (1998)

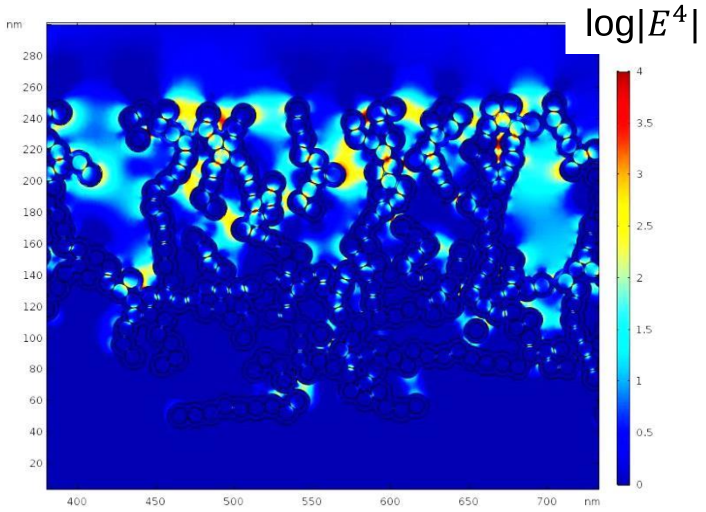
Refractive index of gold

Wavelength	Refractive index
7.80E-07	4.61086642
7.85E-07	4.65225188
7.90E-07	4.69352994
7.95E-07	4.73470422
8.00E-07	4.77577819

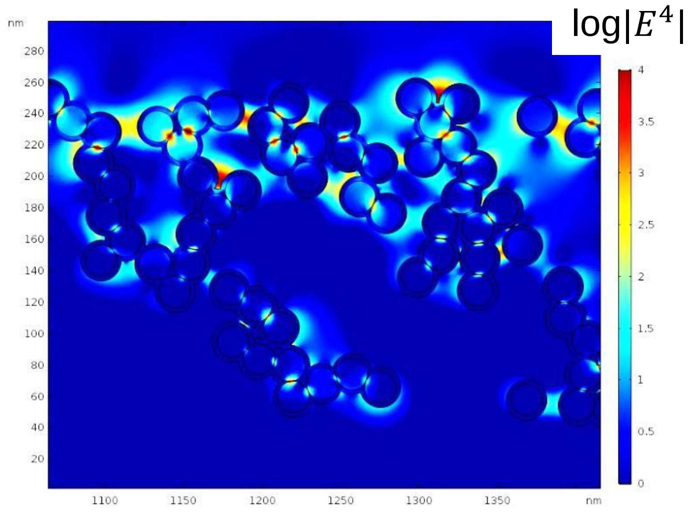
01

Absorption spectra of SERS substrate with various silica primary particles sizes.





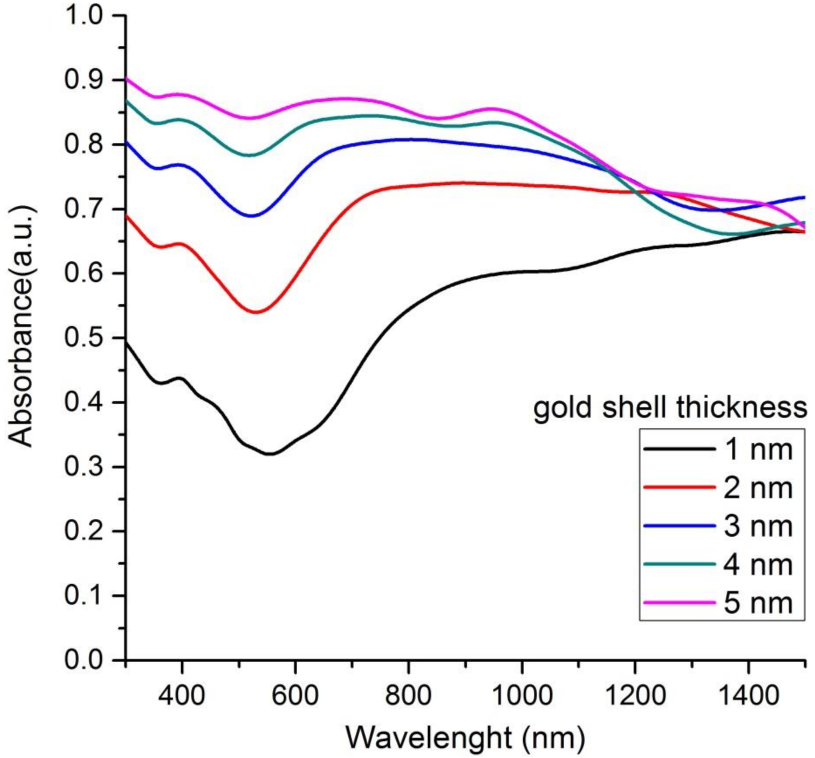
Fill factor = 0.3
Particles diameter = 10 nm
Gold thickness = 3 nm

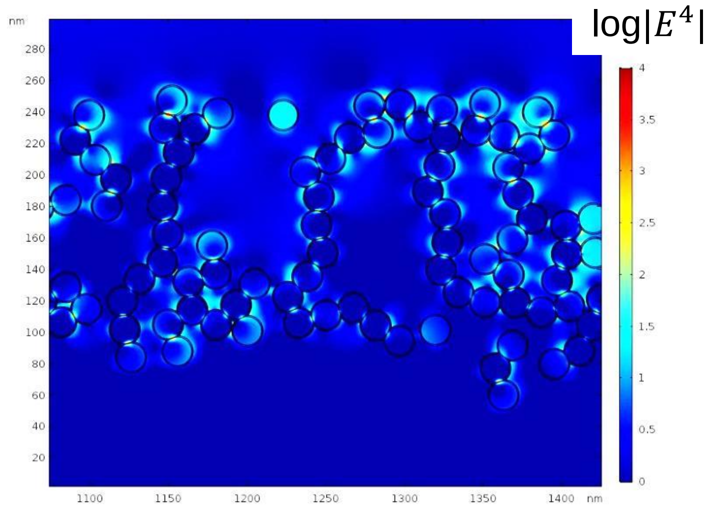


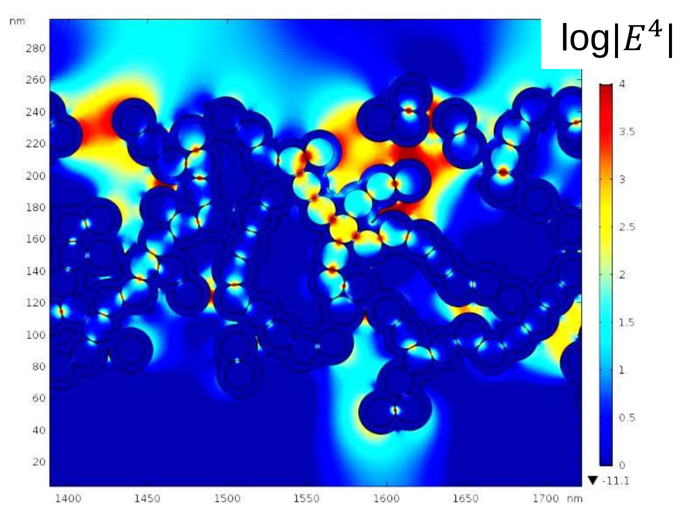
Fill factor = 0.3
Particles diameter = 20 nm
Gold thickness = 3 nm

02

Absorption spectra of SERS substrate with various thickness of coated gold layer.



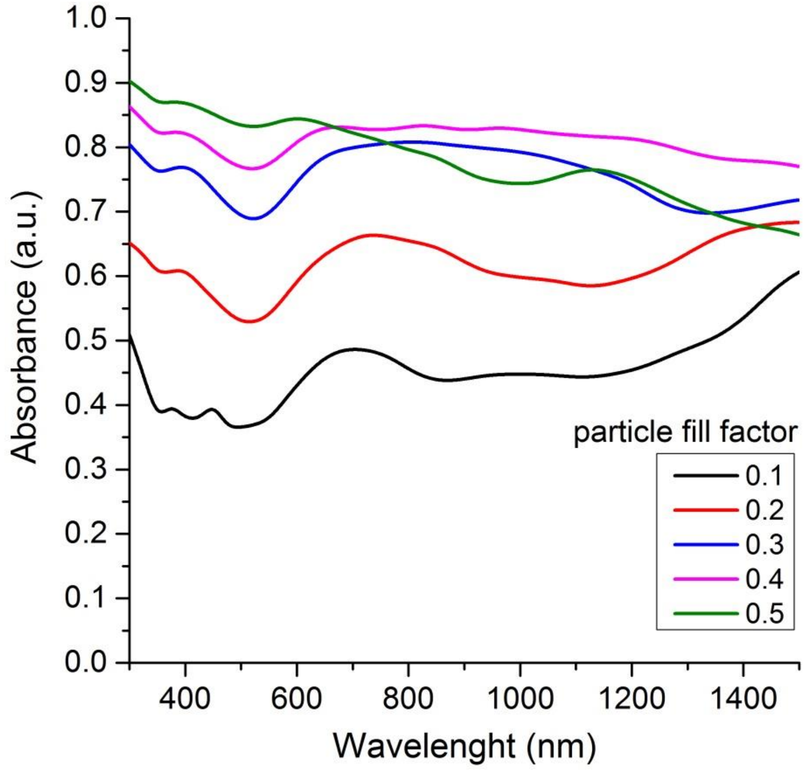


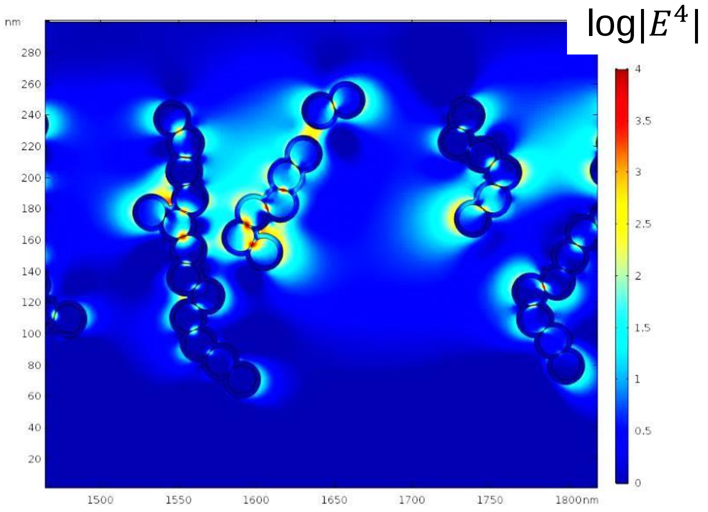


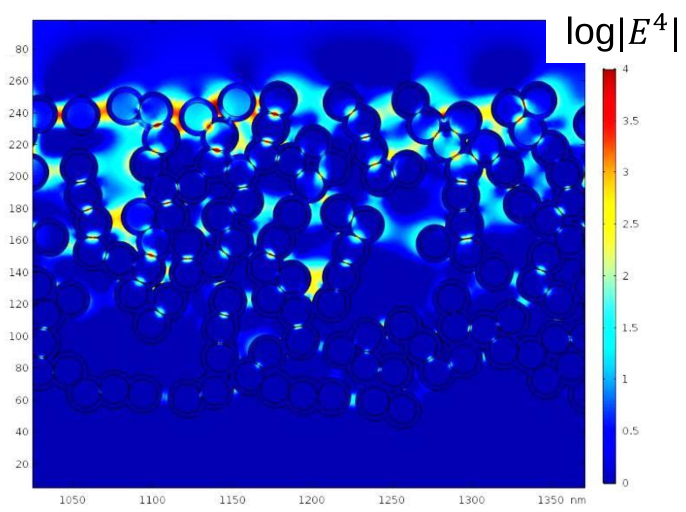
Fill factor = 0.3
Particles diameter = 18 nm
Gold thickness = 1 nm

Fill factor = 0.3
Particles diameter = 18 nm
Gold thickness = 5 nm

03 Absorption spectra of SERS substrate with various packing density of silica particles.

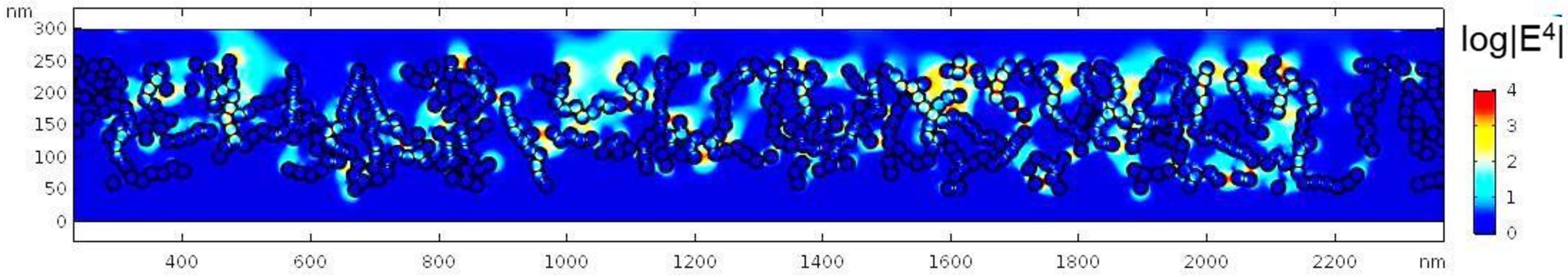




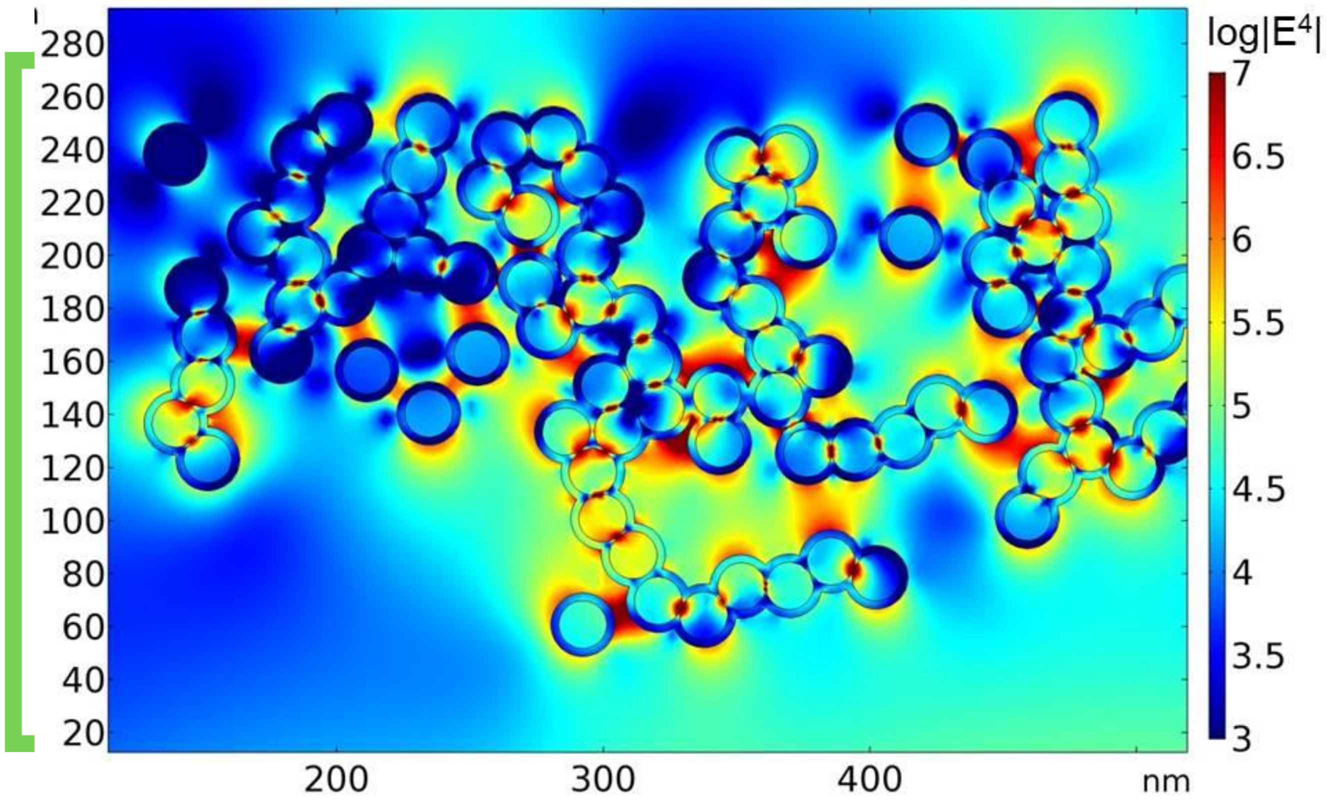


Fill factor = 0.1
Particles diameter = 18 nm
Gold thickness = 3 nm

Fill factor = 0.5
Particles diameter = 18 nm
Gold thickness = 3 nm



The simulation result shows $|E|^4$ distribution on a SERS substrate, excited by a vertical wave incident.



SERS enhancement factor map shows strong field localization at high density of nanogaps

Conclusion

- ❑ COMSOL® program can be use to simulate electric field and optical spectrum of complex plasmonic structure.
- ❑ The numerical results confirm that most of the geometry structures support strong LSPR in NIR spectrum range
- ❑ The optimized structure involves primary silica diameter 18 nm, gold thickness 3 nm, packing density 0.3, which yields enhancement up to 10^7

Future work

- ❑ Need to compare the results with the experiment.

Acknowledgements

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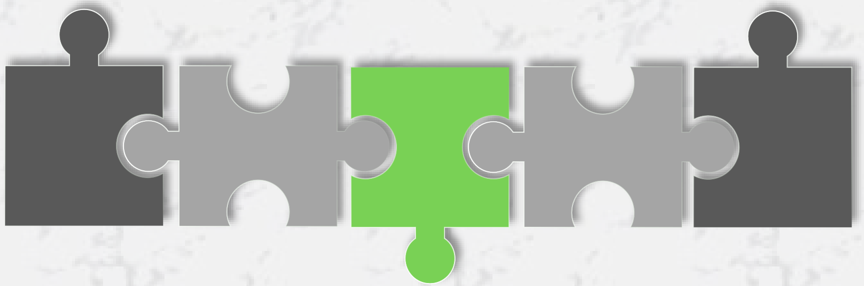
- Department of Physics, Faculty of Science, Prince of Songkhla University
- COMSOL ® Multiphysics



Thank You

For your attention