Antenna and Plasmonic Properties of Scanning Probe Tips at Optical and Terahertz Regimes

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McGill

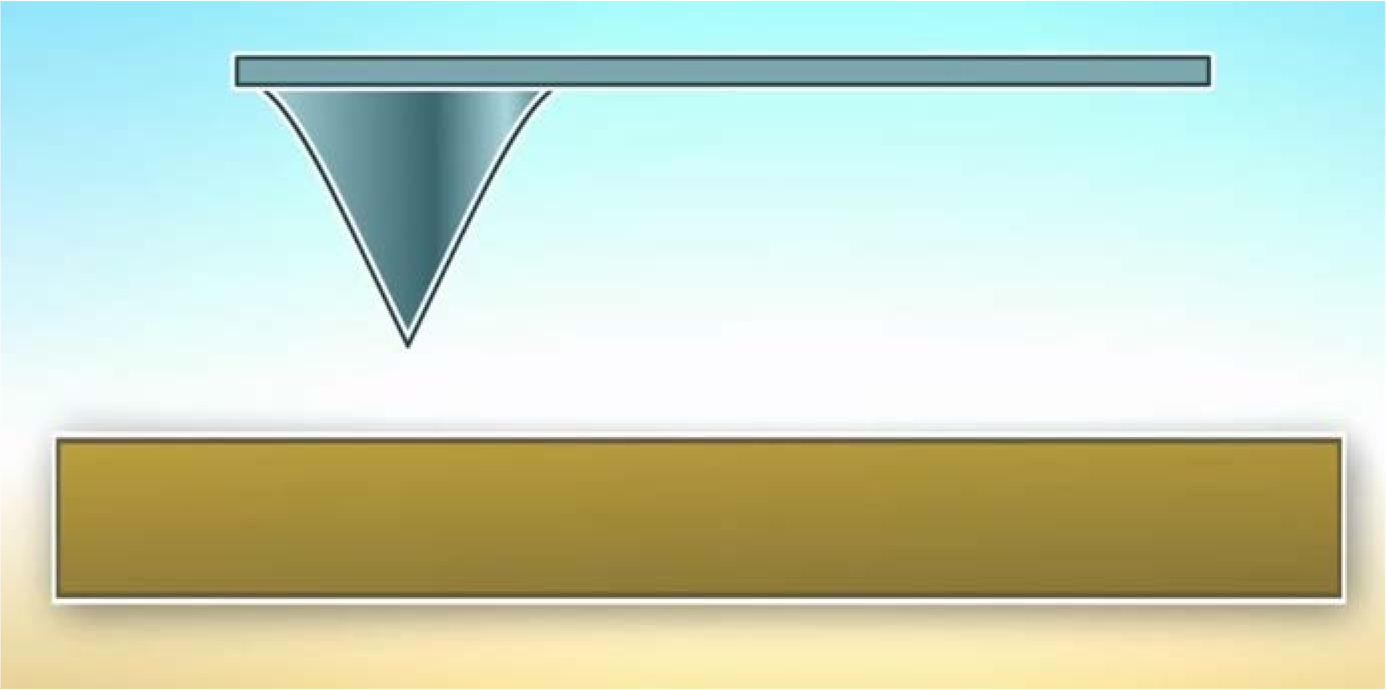
COMSOL CONFERENCE 2014 BOSTON

Outline

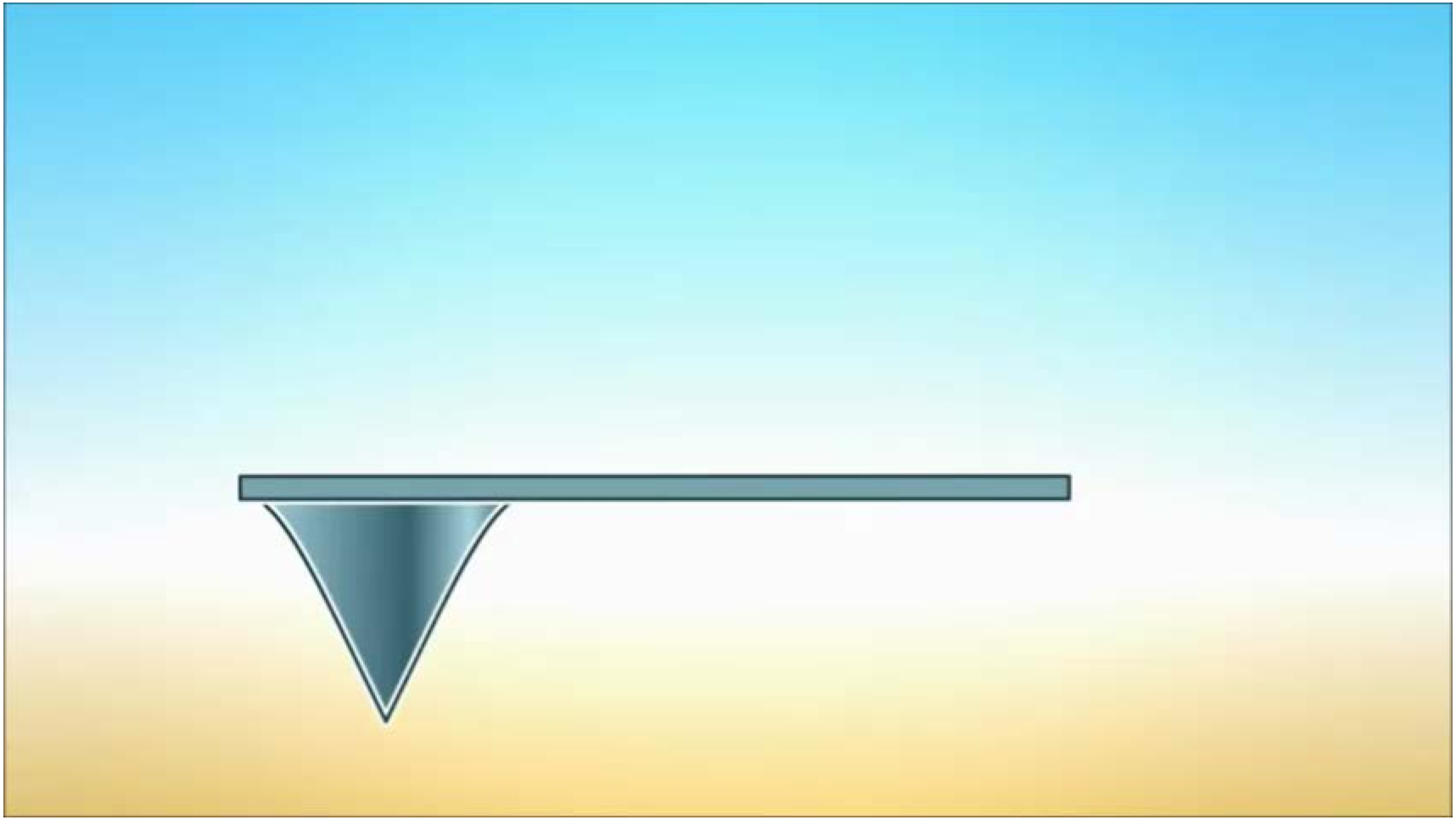
- Introduction
- Analytical theory for full ellipsoid
- COMSOL Multiphysics simulation for Au hemi-ellipsoid
- Computational method
- Results
- Conclusion
- Outlook

Introduction

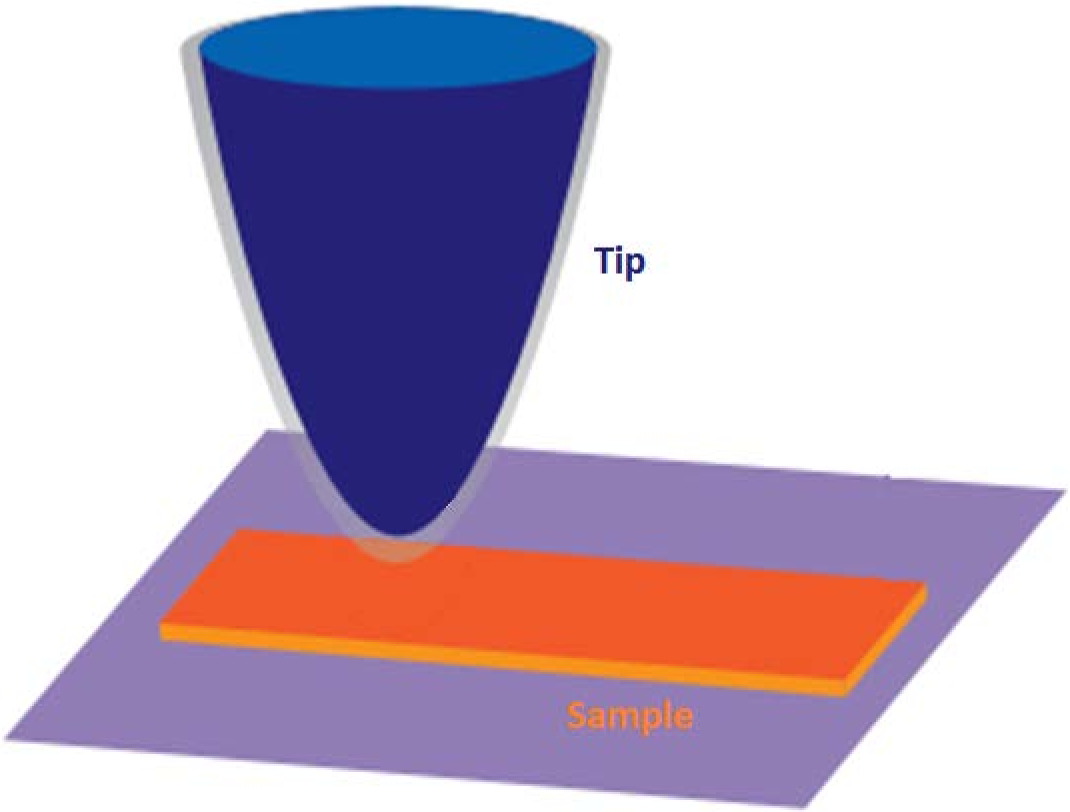
Scanning probe microscopy



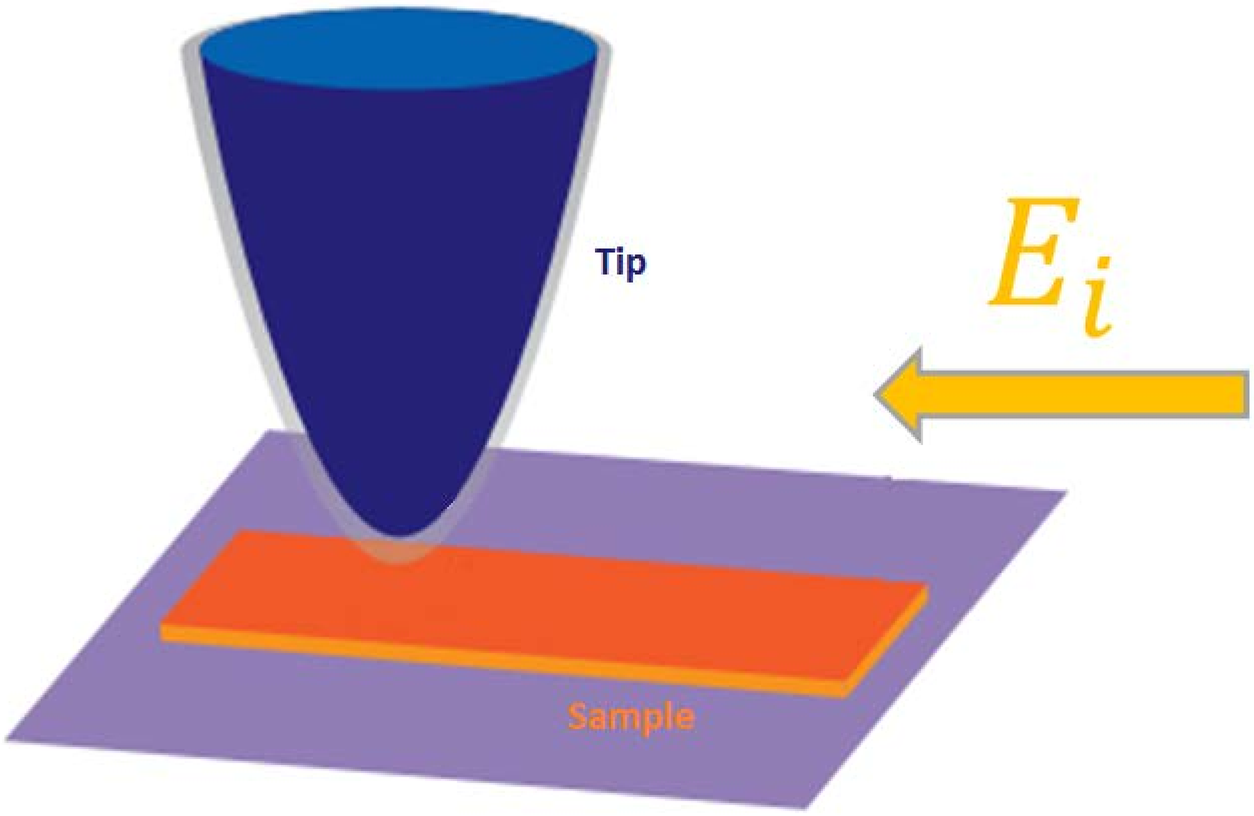
Introduction



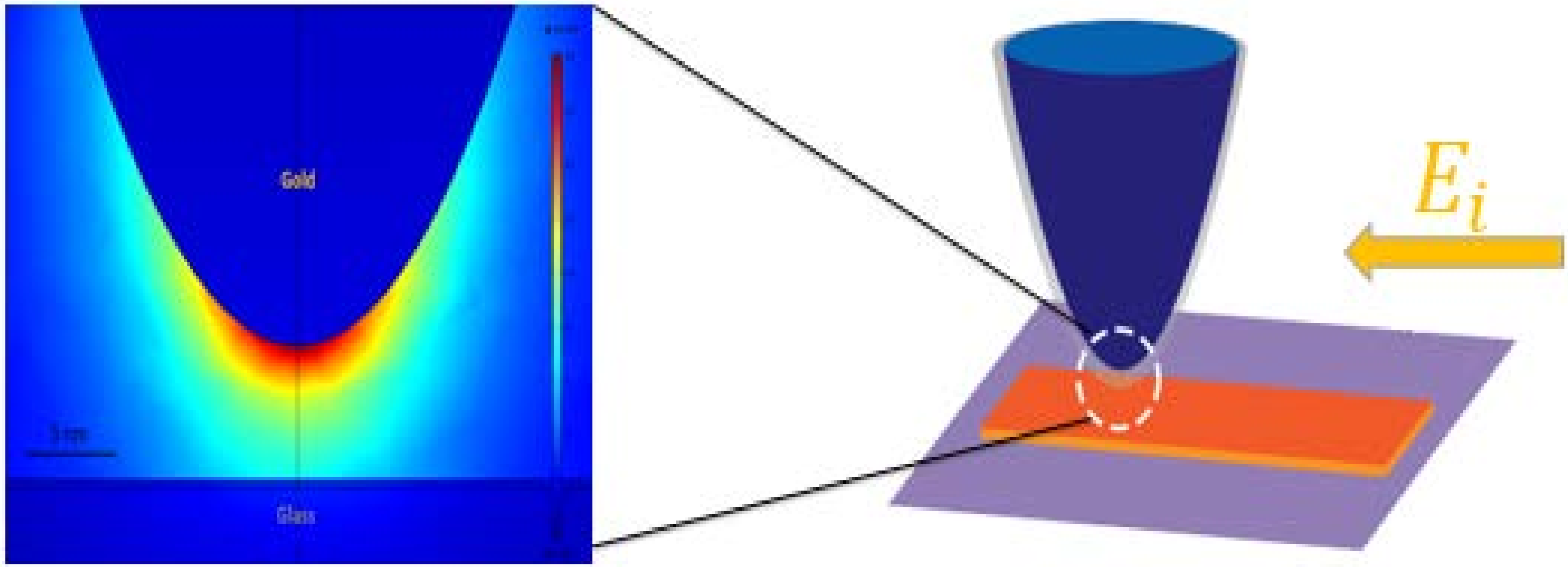
Introduction



Introduction



Introduction



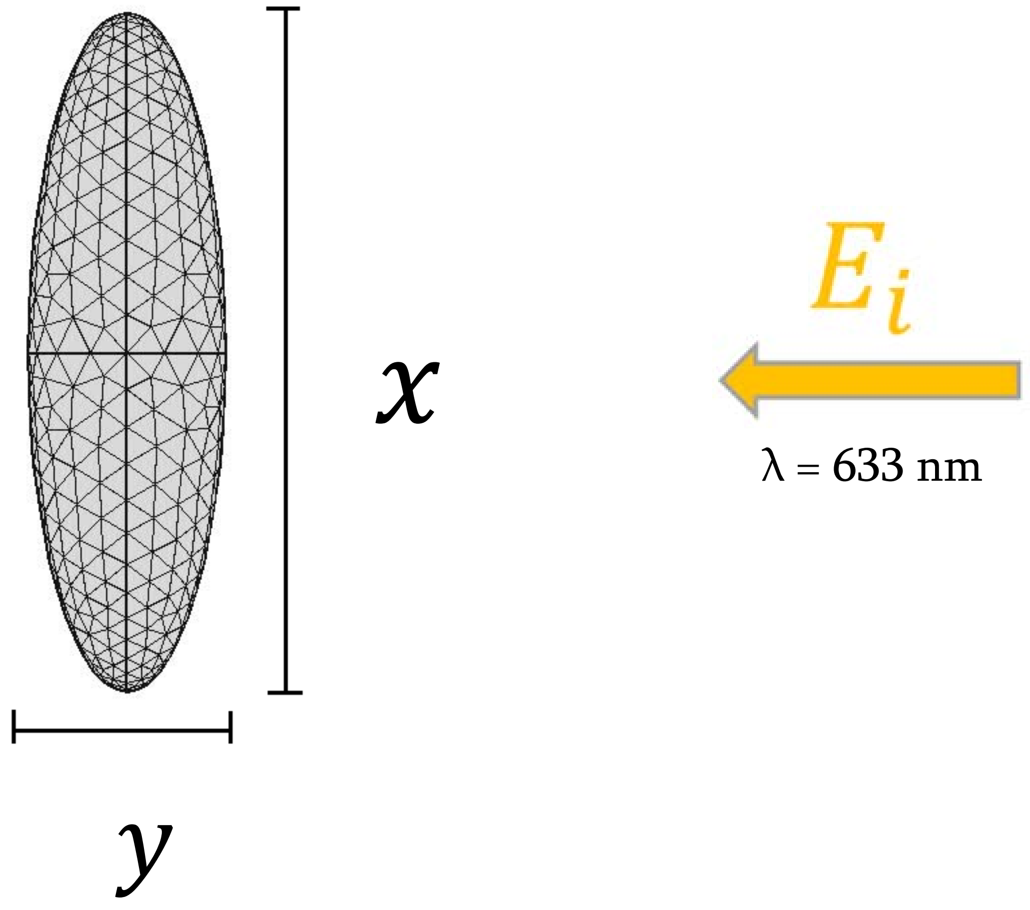
Introduction

- **Questions:**

  - Physics behind the electric field enhancement at the end of a sharp tip?
  - Which parameters can effect the enhancement of electric field ?

Analytical theory for full ellipsoid

$$r = \frac{x}{y}$$



Analytical theory for full ellipsoid

- Field enhancement factor

Frequency dependence

$$\gamma = \left|\frac{\varepsilon}{1 + (\varepsilon - 1)A}\right|$$

Geometrical dependence

- Depolarization factor

$$A(r) = \frac{1}{2r^2}\int_0^\infty \frac{1}{(s+1)^{\frac{3}{2}}\,(s+r^{-2})}\,ds$$

- Permittivity

$$\varepsilon\,(\omega) = \varepsilon'\,(\omega) - j\varepsilon''\,(\omega)$$

Plasmon and antenna effects are included

Analytical theory for full ellipsoid

Antenna resonance :

Odd integer multiple of half a wavelength

$$x = n\lambda + \frac{\lambda}{2}$$

n= 0,1,2,…

Analytical theory for full ellipsoid

Antenna resonance :

Finite Element Time Domain (FETD) calculations

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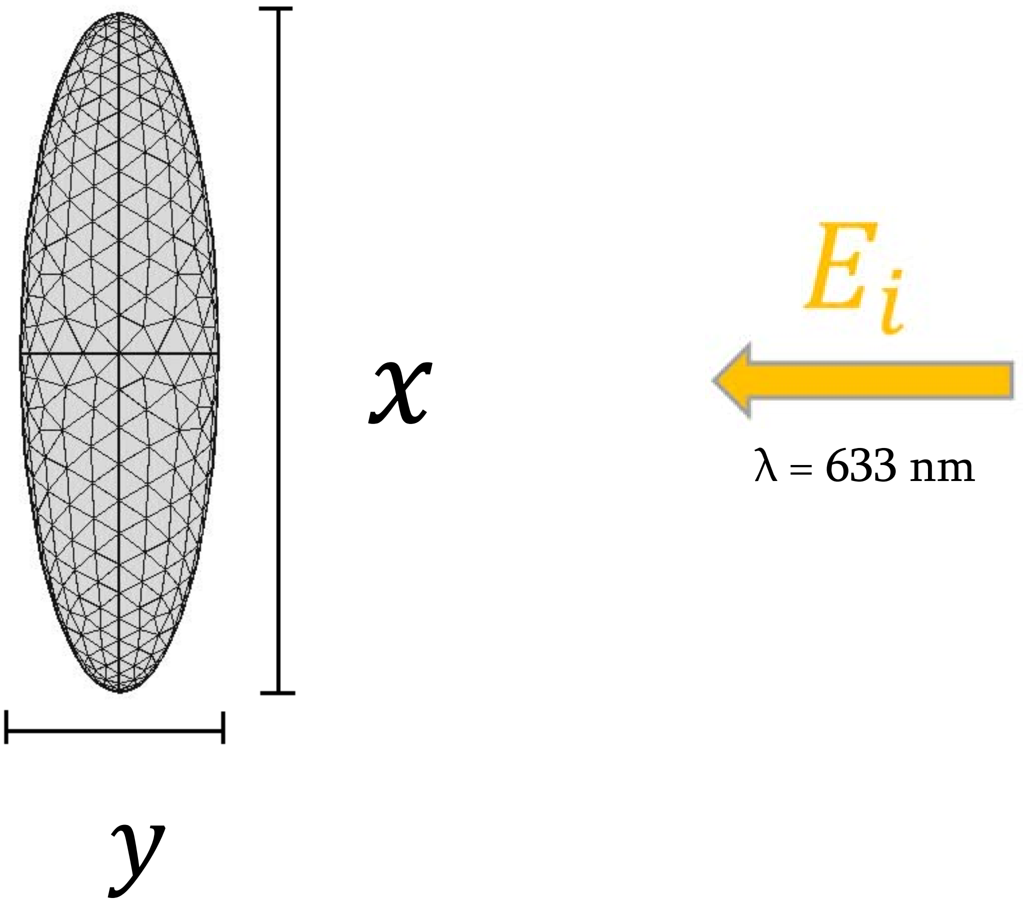
FETD



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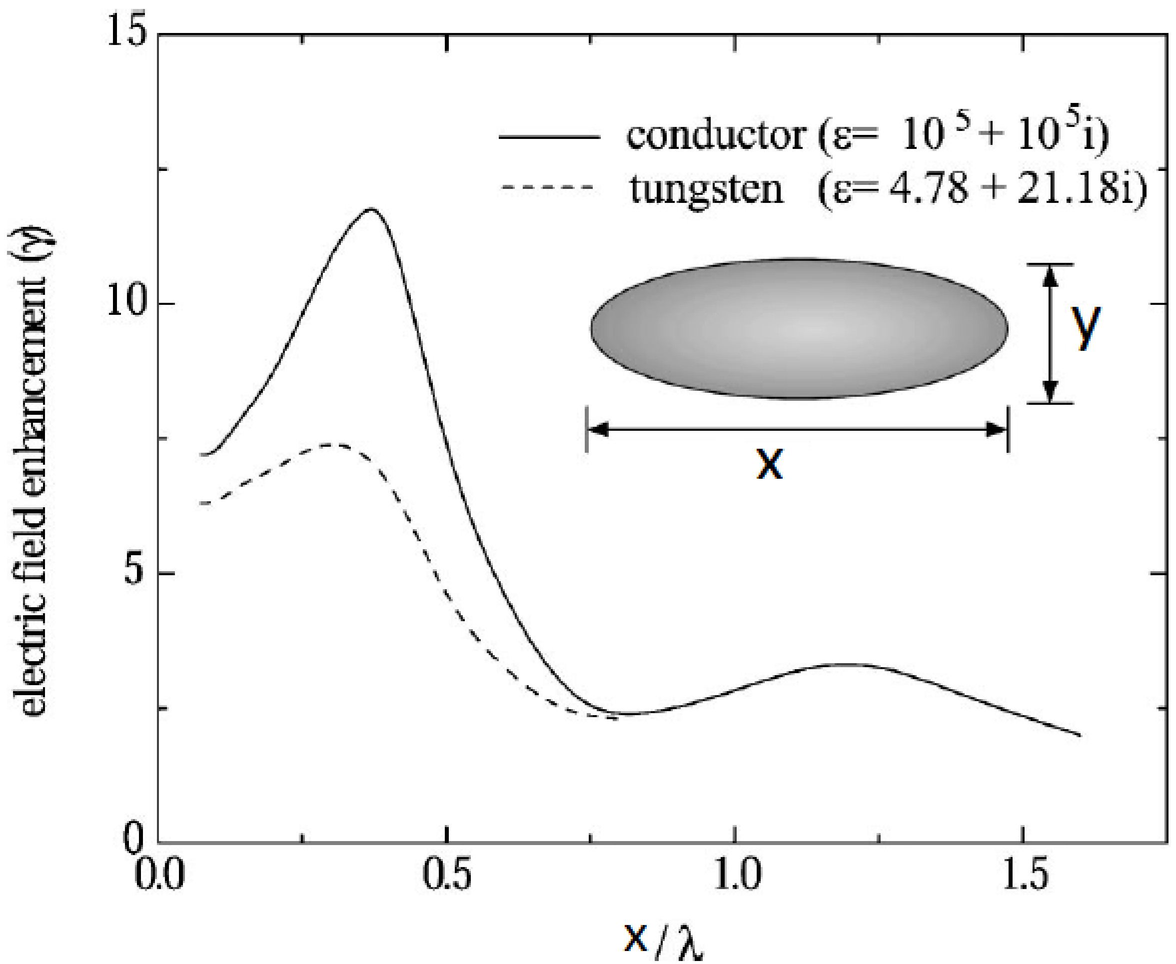
FETD

- Antenna resonance

$\lambda = 633$ nm

$$x = n\lambda + \frac{\lambda}{2}$$

$r = x/y = 3$



Calculated field enhancement at the end of small ellipsoid. Dephasing effects reduce the field enhancement for a greater than 0.5 λ

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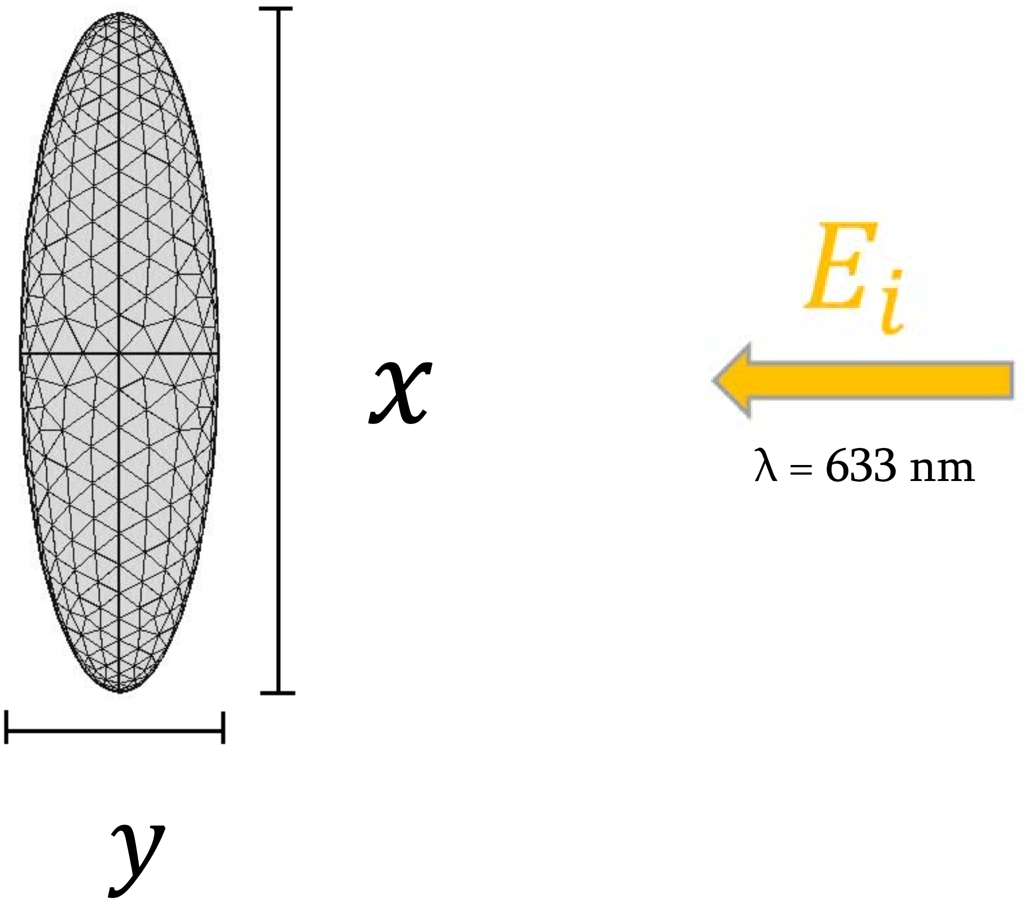
Analytical theory for full ellipsoid

Plasmon resonance :

$$\gamma = \left|\frac{\varepsilon}{1 + (\varepsilon - 1)A}\right|$$

$$Re[1 + (\varepsilon(\omega) - 1)A] = 0$$

FETD



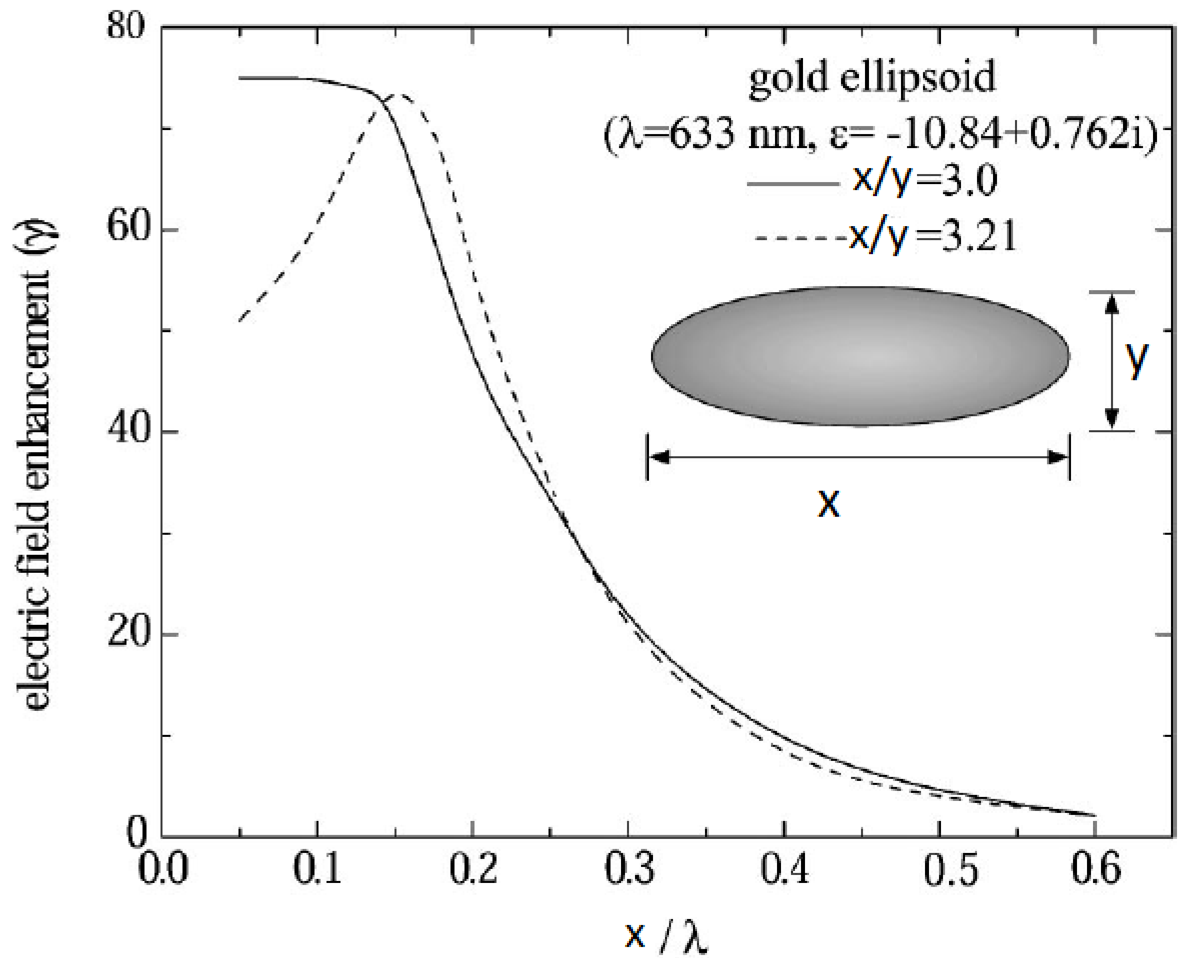
FETD

- Plasmon resonance:

$$Re[1 + (\varepsilon(\omega) - 1) \times A] = 0$$

$$A(r) = \frac{1}{2r^2} \int_0^\infty \frac{1}{(s+1)^{\frac{3}{2}}\ (s + r^{-2})}\, ds$$

$$r = \frac{x}{y} = 3.2$$



Calculated field enhancement for gold ellipsoid at 633 nm. Very large enhancements are found for small size, due to plasmon resonance. Values calcuated agree resonably well with analytical resutls at small sizes. Dephasing effects drastically decrease at larger size. When X is greater than 0.5λ, field enhancement is smaller than 5

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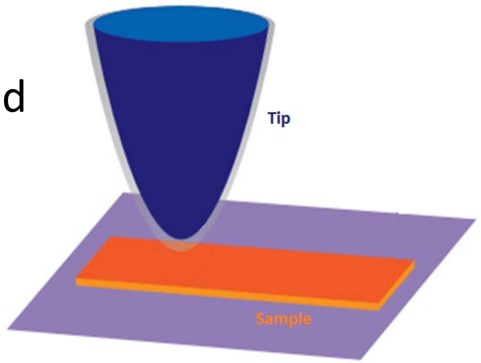
But!



The tip apex is not a full ellipsoid but a hemi-ellipsoid

↓

Modeling the tip as Au hemi-ellipsoid

↓

Solving the Maxwell equations in frequency domain

↓

Finite Element Method (FEM) using COMSOL Multiphyiscs

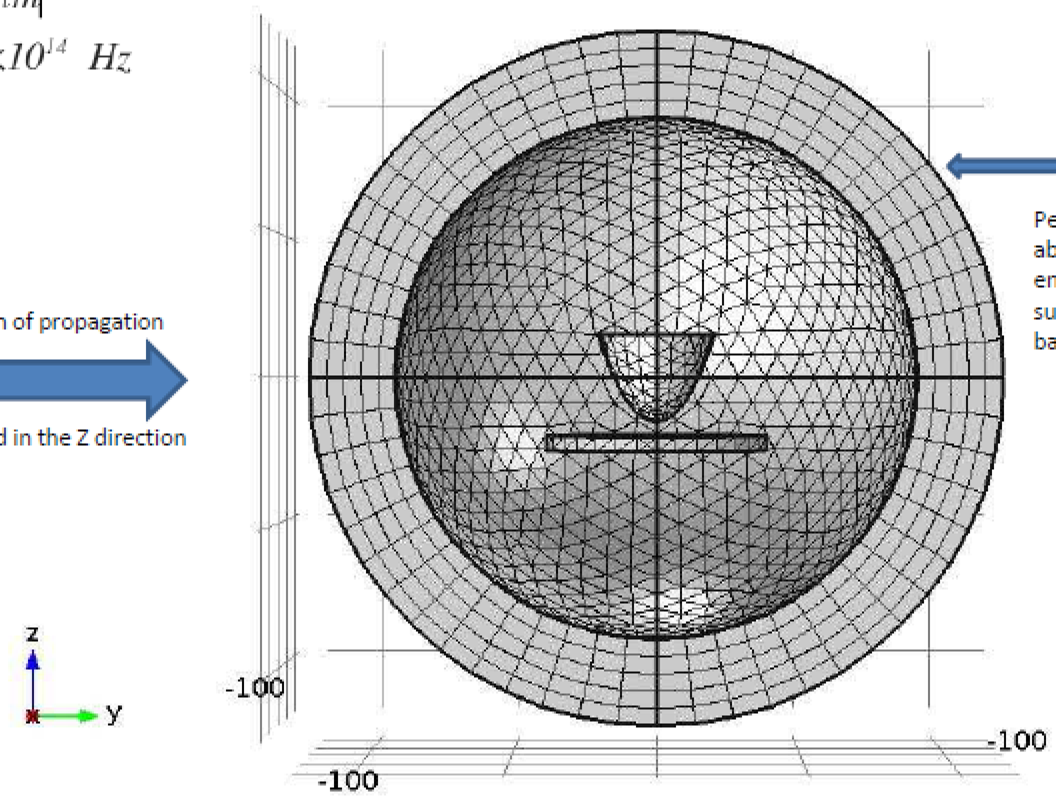
COMSOL simulation for Au hemi-ellipsoid

$\lambda = 630\ nm$

$\upsilon = 4.76 \times 10^{14}\ Hz$

Direction of propagation

Polarized in the Z direction



Perfectly matched layer to absorb the scattered light emitting from the tip apex and substrate (to avoid reflecting back to the system)

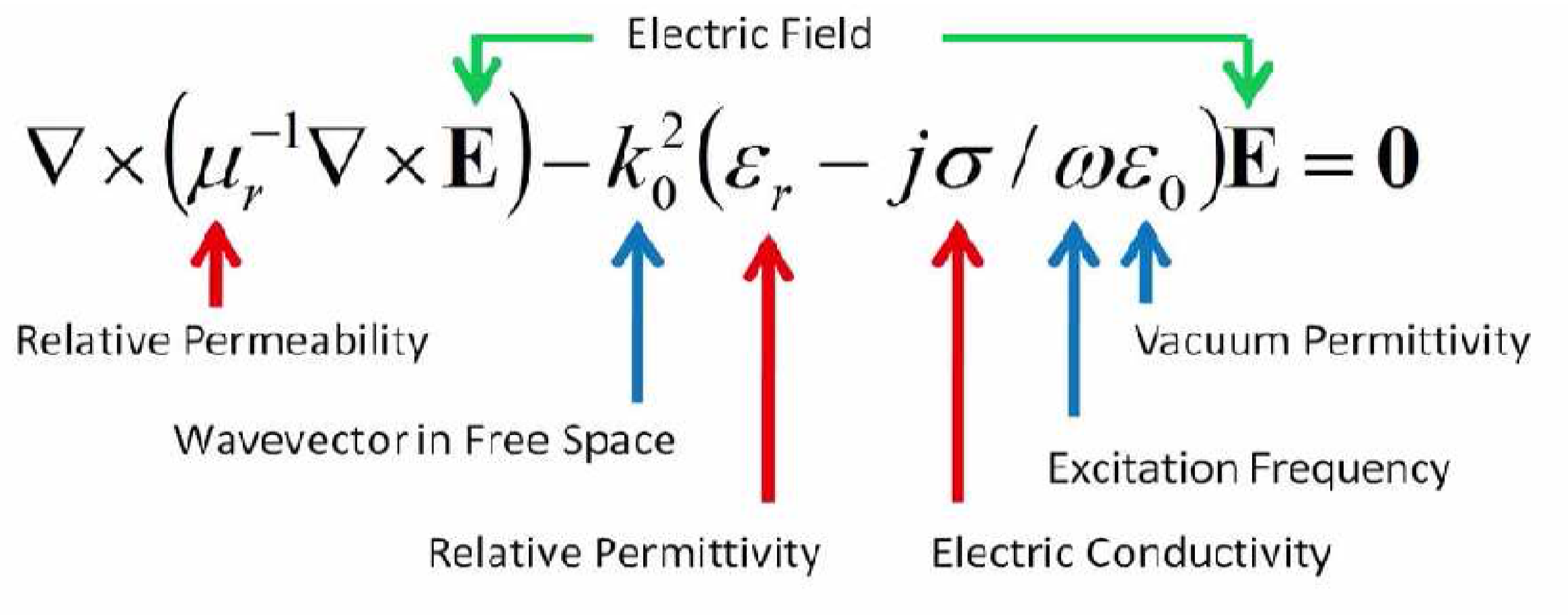
Computational method

Frequency domain form of Maxwell's equations describing the electric fields inside of the domain, at a known excitation frequency

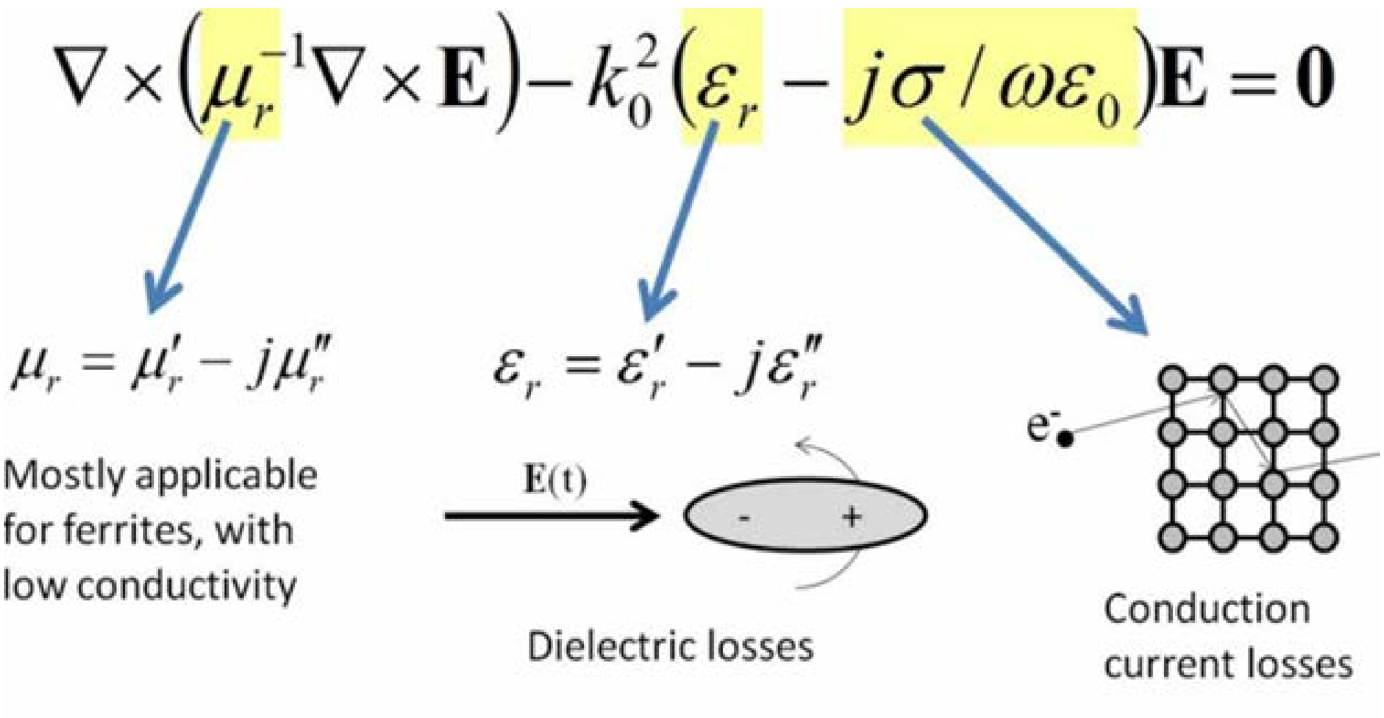
Electric Field

$$\nabla \times \left(\mu_r^{-1} \nabla \times \mathbf{E}\right) - k_0^2 \left(\varepsilon_r - j\sigma / \omega\varepsilon_0\right)\mathbf{E} = \mathbf{0}$$

COMSOL simulation for Au hemi-ellipsoid



Loss terms:


$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k_0^2 (\varepsilon_r - j\sigma / \omega\varepsilon_0)\mathbf{E} = \mathbf{0}$
$\mu_r = \mu_r' - j\mu_r''$
$\varepsilon_r = \varepsilon_r' - j\varepsilon_r''$
Mostly applicable for ferrites, with low conductivity
E(t)
-
+
Dielectric losses
e-
Conduction current losses

COMSOL simulation for Au hemi-ellipsoid

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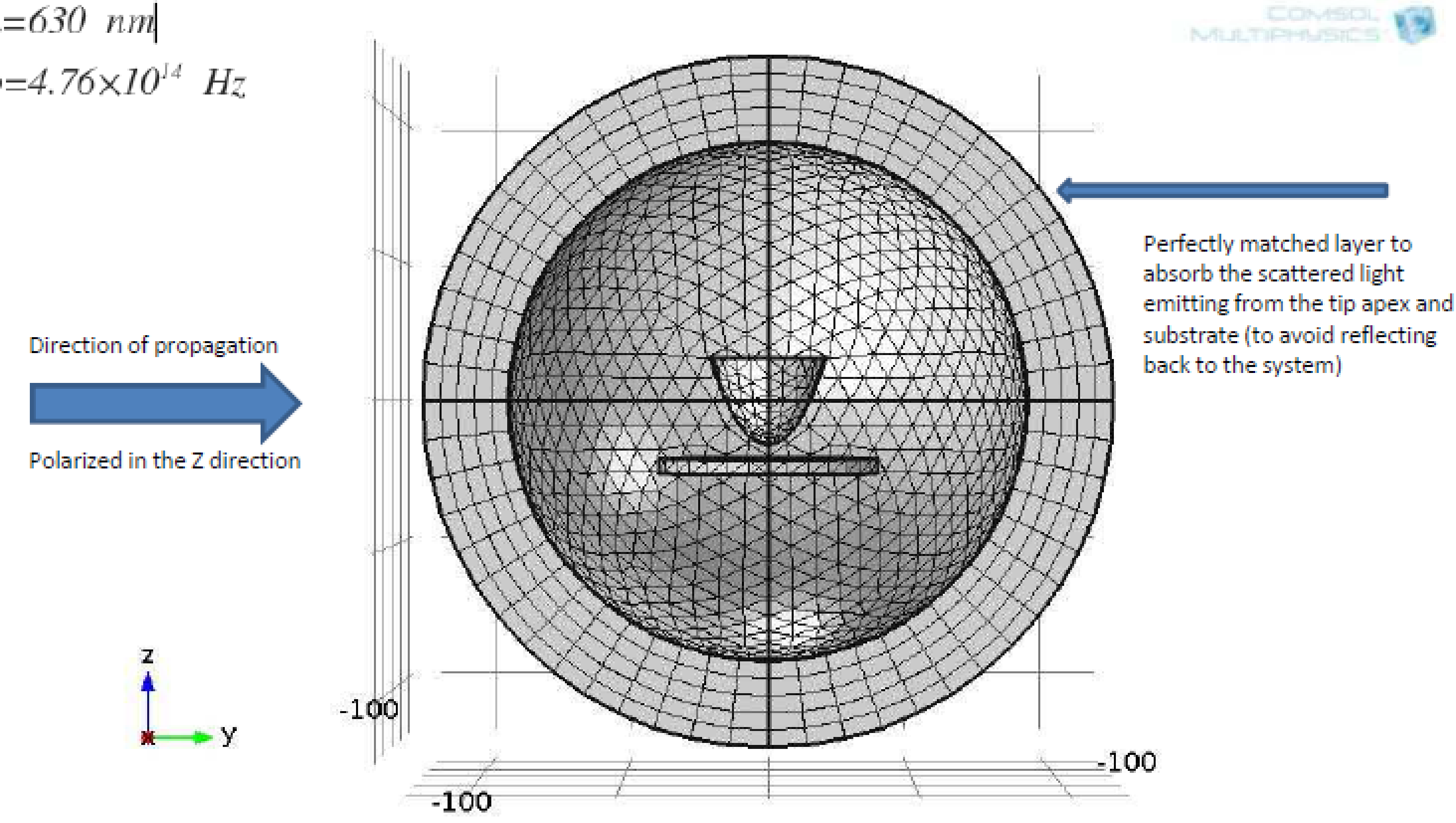
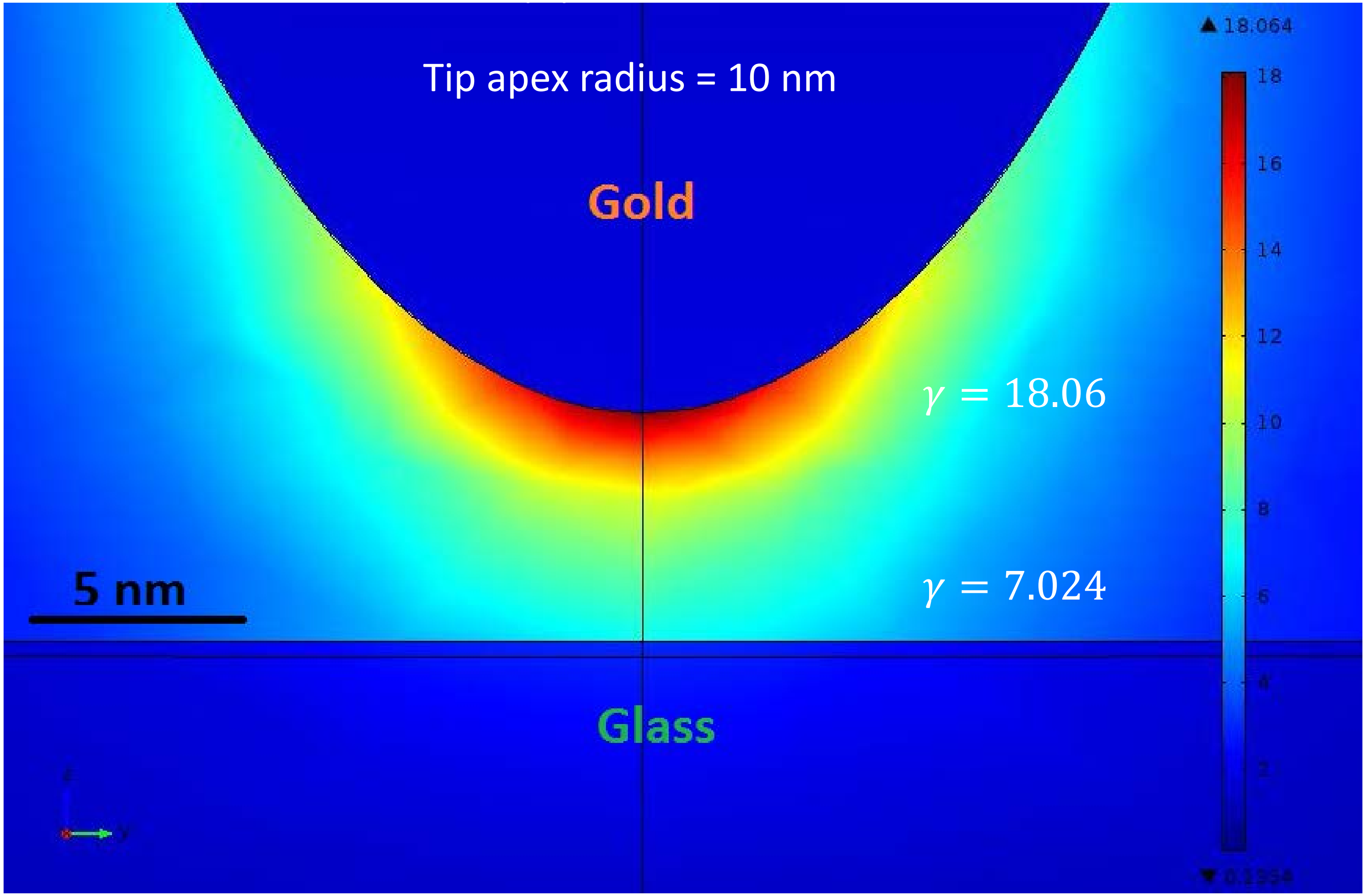


Perfectly matched layer to absorb the scattered light emitting from the tip apex and substrate (to avoid reflecting back to the system)

COMSOL simulation for Au hemi-ellipsoid

Result:



COMSOL simulation for Au hemi-ellipsoid

Comparing the result:

TABLE 1: Field Enhancement near the Sample Surface Plane at $z = 0.125$ nm and $x = 0$ nm for Different Tip−Substrate Material Combinations for Tips with $R = 10$ nm and $\theta = 45°$ at $d = 5$ nm

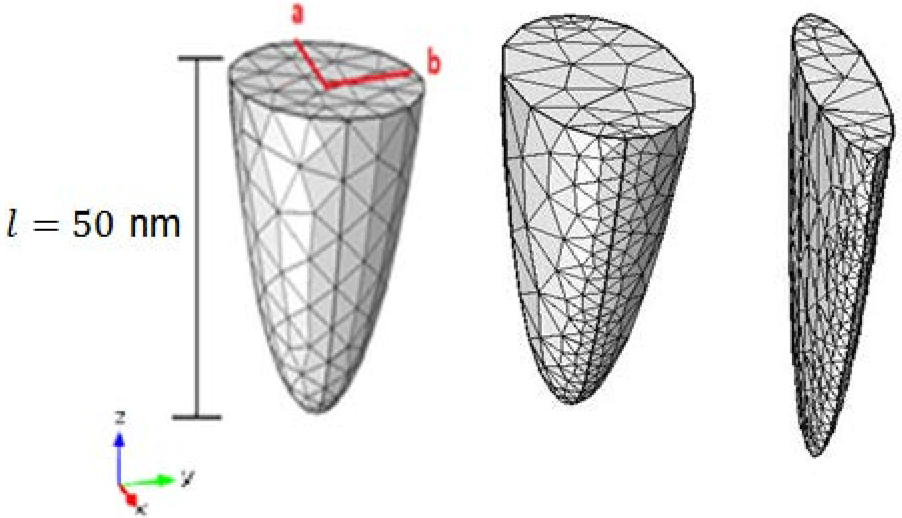
surface	Au tip	W tip	Si tip	glass tip
Au	49.8	14.2	9.2	2.5
W	25.4	10.1	7.1	2.3
Si	19.6	8.7	6.2	2.2
glass	8.4	5.0	3.9	1.8

J. Phys. Chem. C **2008**, *112*, 3766−3773

COMSOL simulation for Au hemi-ellipsoid

Which parameters can effect the enhancement of electric field?

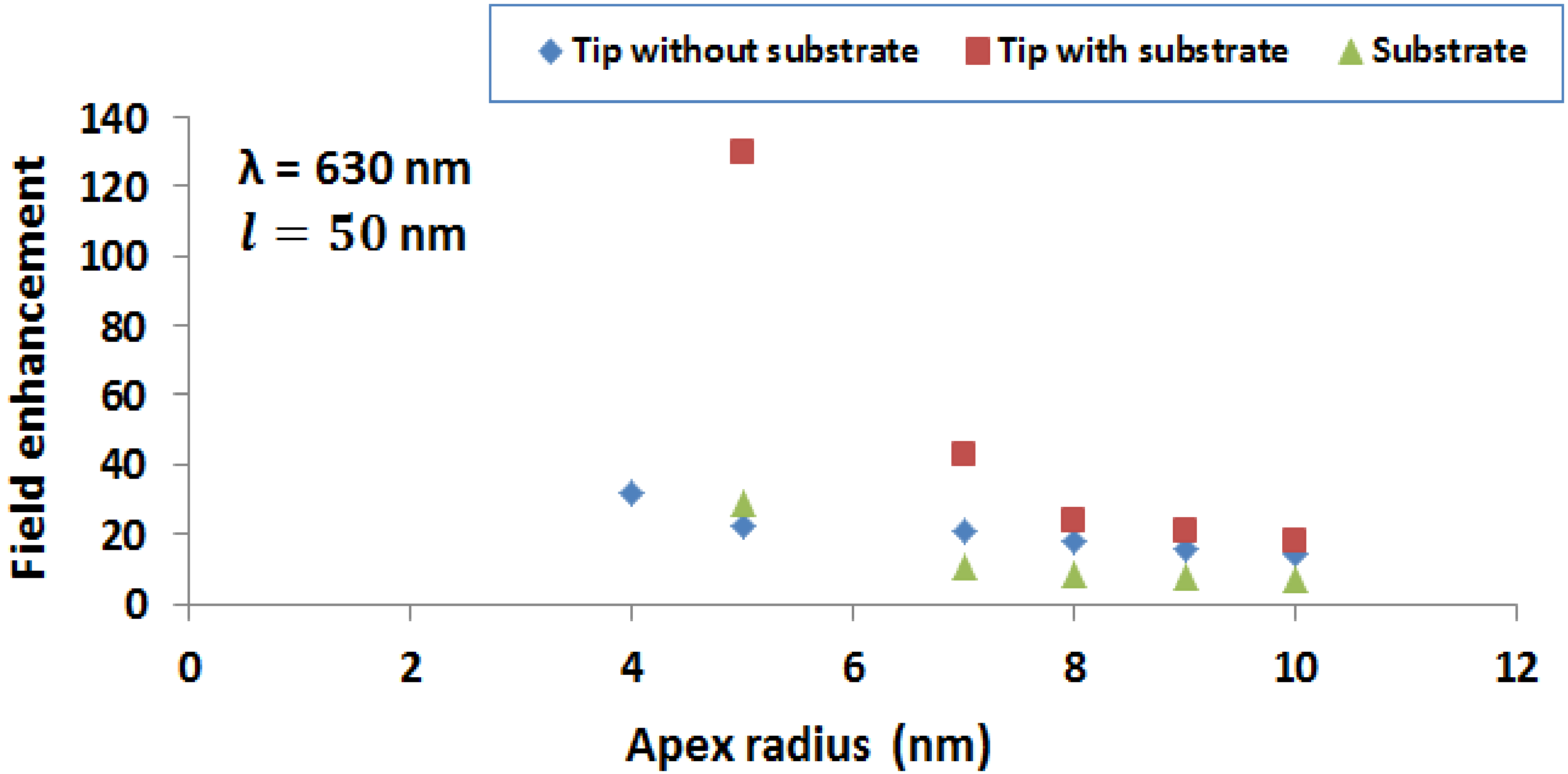
- Apex radius
- Substrate
- Radiation wavelength
- Tip-sample distance
- Tip and substrate material
- Geometrical shape
- Tip and substrate materials



COMSOL simulation for Au hemi-ellipsoid

- Dependence of electric field enhancement at optical regime on the apex radius with and without substrate

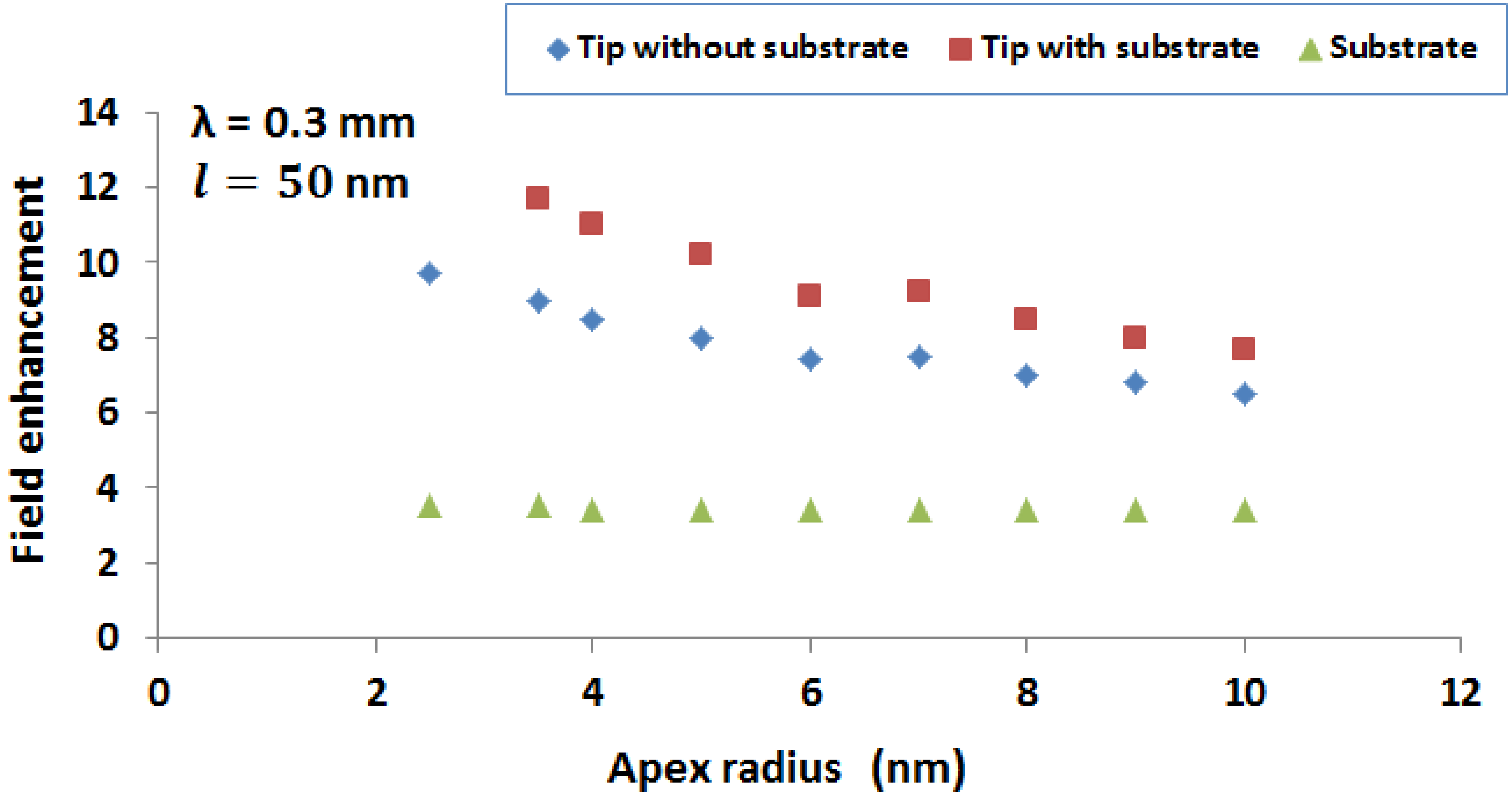
$$\varepsilon_{Optic} = -9.90 + 1.05\, i$$



COMSOL simulation for Au hemi-ellipsoid

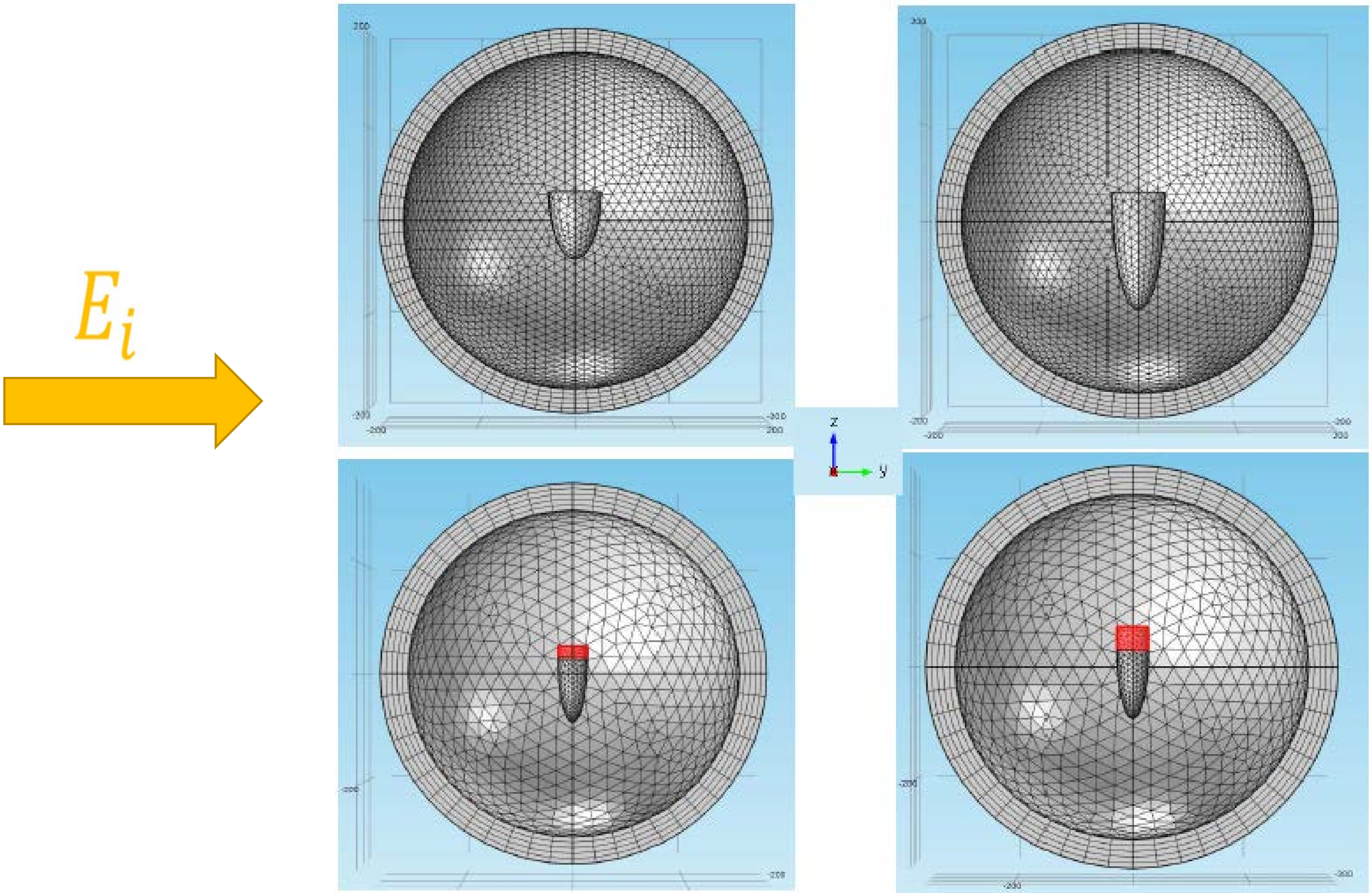
- Dependence of electric field enhancement at THz regime on the apex radius with and without substrate

$$\varepsilon_{THz} = -1.4 \times 10^5 + 1.6 \times 10^6\, i$$



COMSOL simulation for Au hemi-ellipsoid

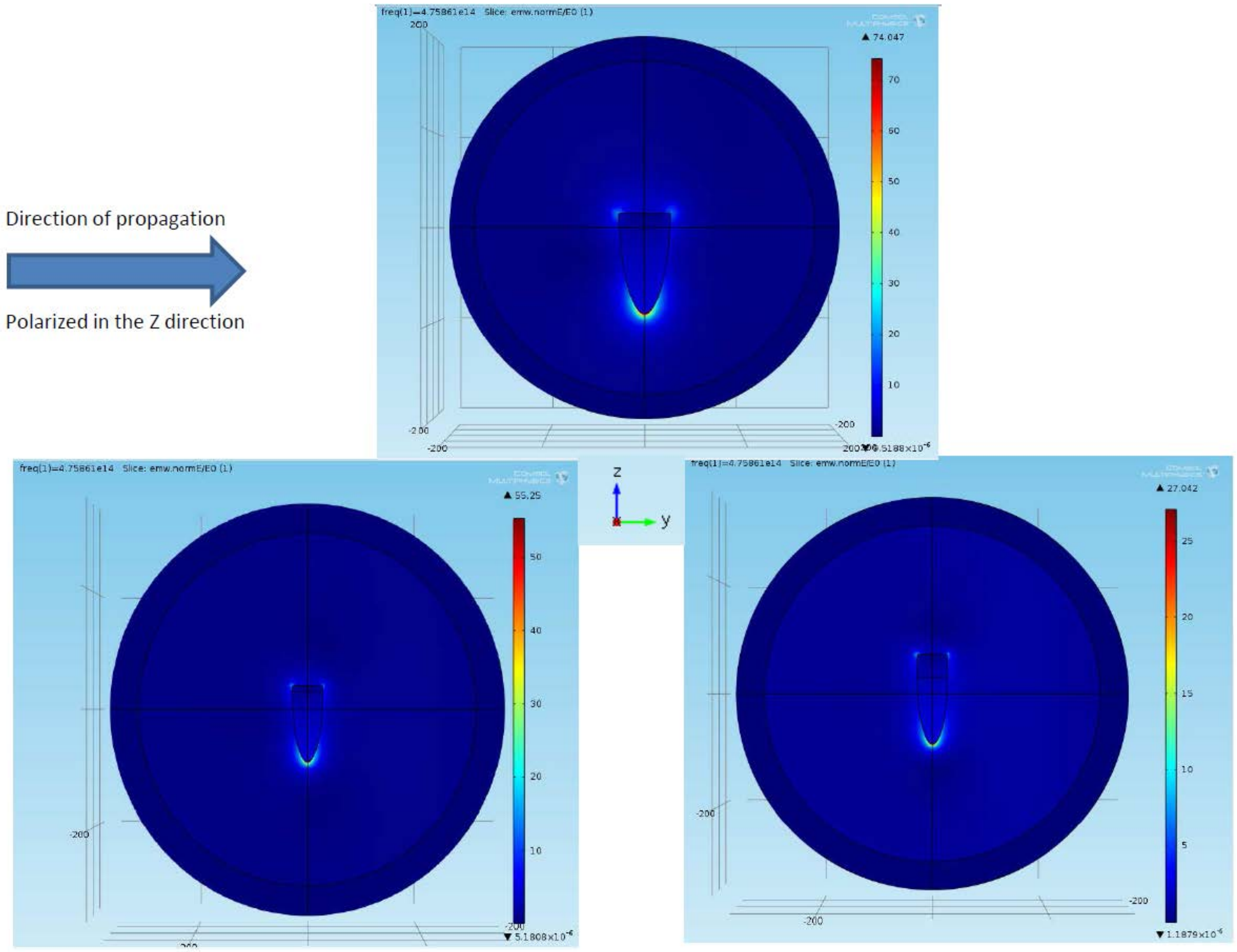
Antenna and plasmonic properties?



COMSOL simulation for Au hemi-ellipsoid

Antenna and plasmonic properties with associated dephasing effects?

Result:



COMSOL simulation for Au hemi-ellipsoid

Antenna and plasmonic properties with associated dephasing effects?

Result:

$$\gamma = \left| \frac{\varepsilon}{1 + (\varepsilon - 1)A} \right|$$

$$A(r) = \frac{1}{2r^2} \int_0^\infty \frac{1}{(s+1)^{\frac{3}{2}}\,(s + r^{-2})}\, ds$$

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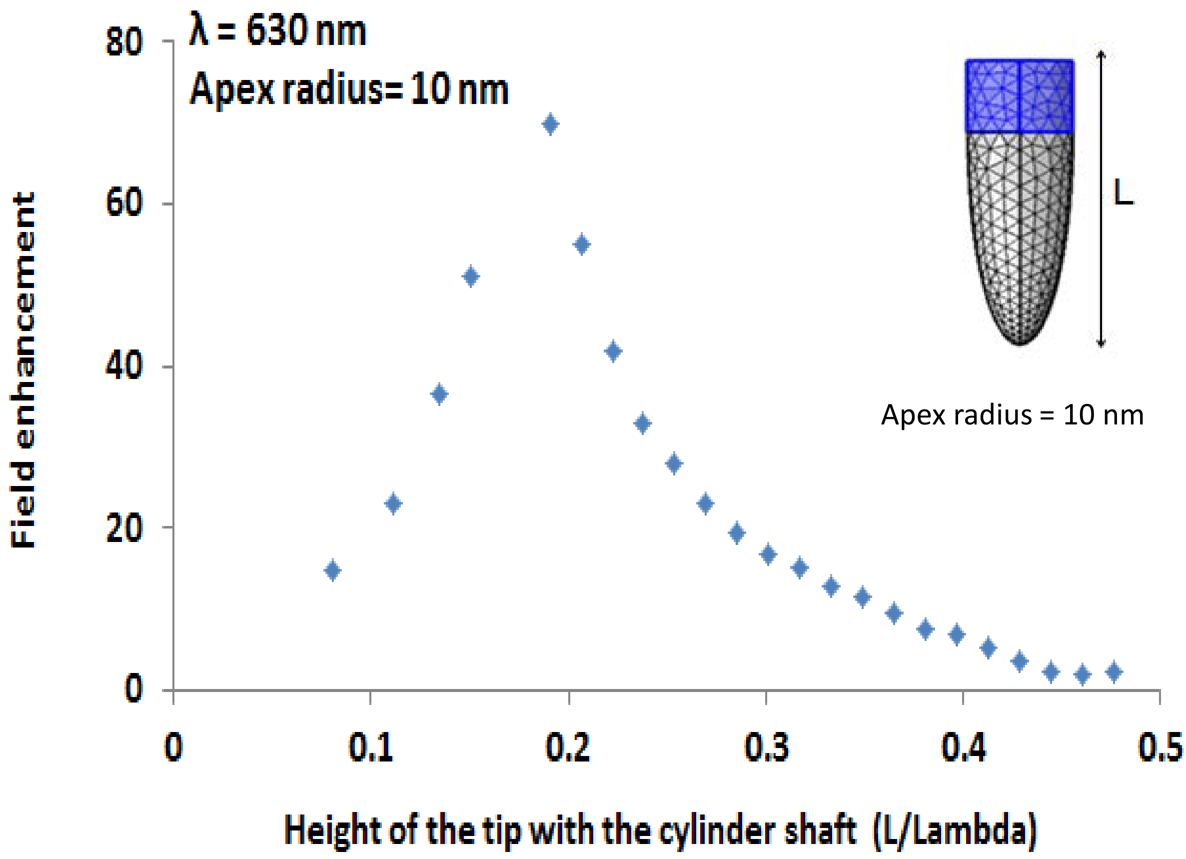

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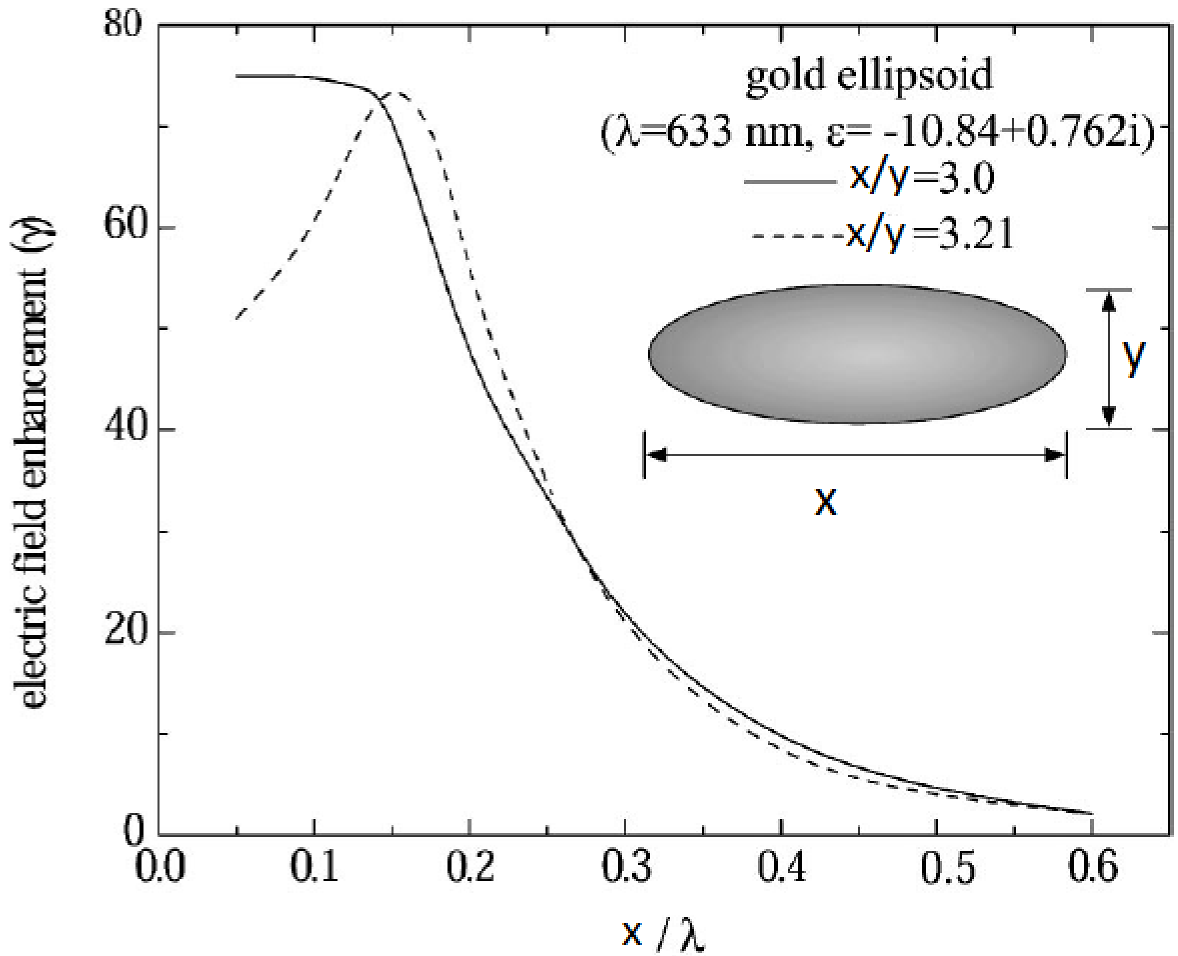

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COMSOL simulation for Au hemi-ellipsoid

- Plasmon resonance for Au hemi-ellipsoid:

$$r = x/y \approx 2$$

COMSOL simulation for Au hemi-ellipsoid

How about THz?

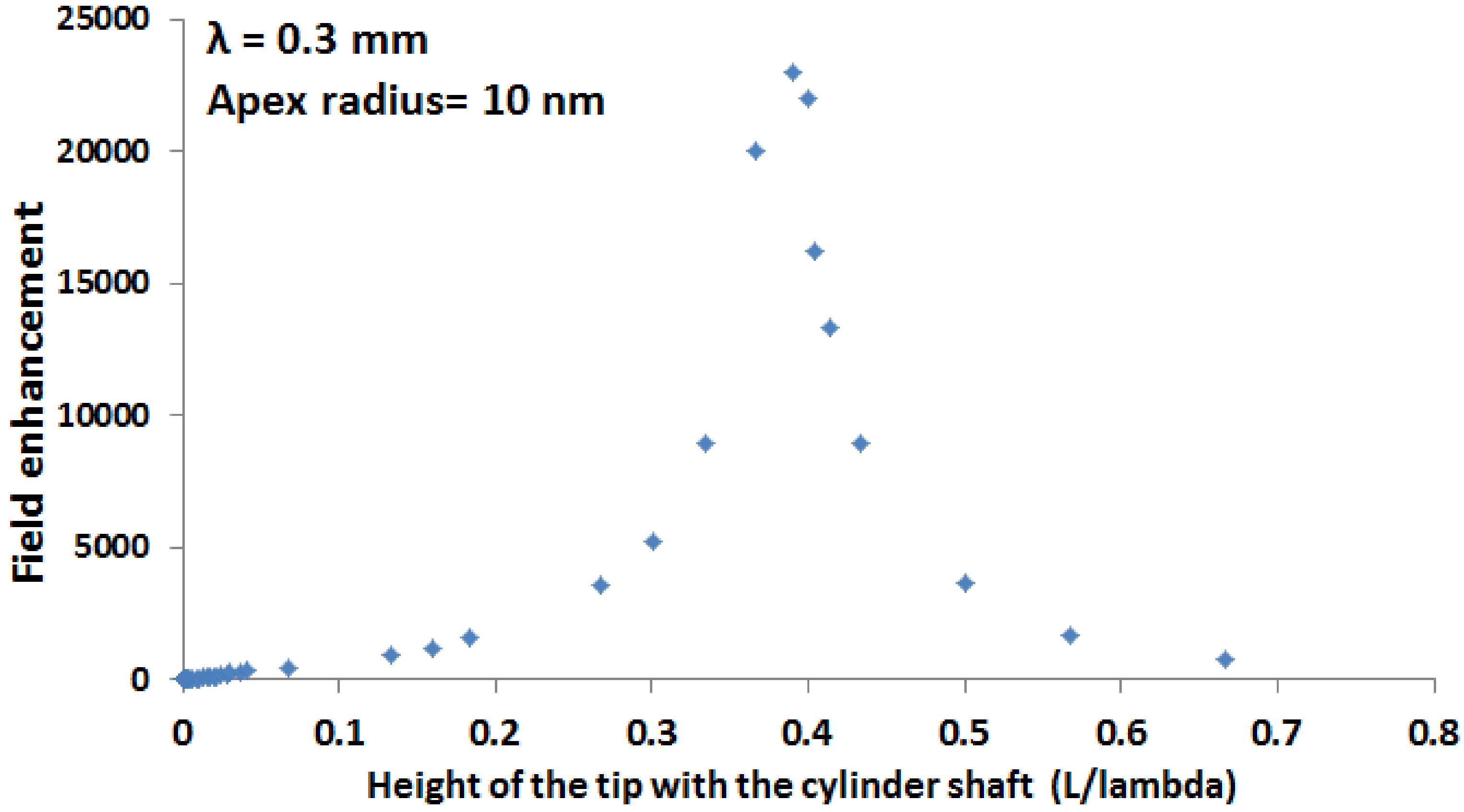
COMSOL simulation for Au hemi-ellipsoid

$$\gamma = \left| \frac{\varepsilon}{1 + (\varepsilon - 1)A} \right|$$

$$A(r) = \frac{1}{2r^2} \int_0^\infty \frac{1}{(s+1)^{\frac{3}{2}}\ (s + r^{-2})}\ ds$$

COMSOL simulation for Au hemi-ellipsoid

Antenna and plasmonic properties with associated dephasing effects?



Conclusion

- Antenna and plasmon resonances are two different underlying physical origins of the field enhancement at the end of a sharp tip.
- Dephasing effects can severely decrease field enhancement at optical regime.
- At THz regime, the antenna effect is dominant leading to an extremely high field enhancement
- For Au hemi-ellipsoid illuminated by λ= 630 nm, plasmon resonance can be obtained when $r \approx 2$
- COMSOL simulation agrees with the analytical results

Outlook

- Combining RF and Heat transfer modules together
- Measuring the total dissipation at the system
- Adding cantilever to the tip
- Coating the tip and cantilever
- …

Acknowledgment

Peter Grutter

Yoichi Miyahara

Group members

Thanks