DPMS: Advanced Materials

LAB E11:
Computational Optics II

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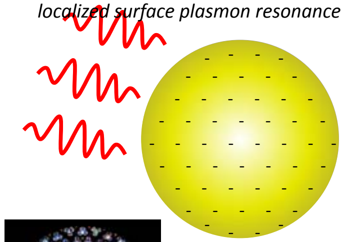
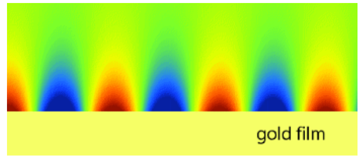
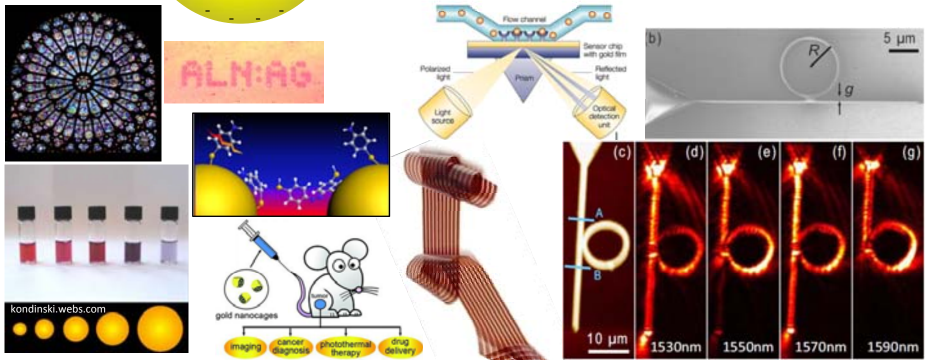
Plasmonics in technology

Localized Plasmons
localized surface plasmon resonance (LSPR)



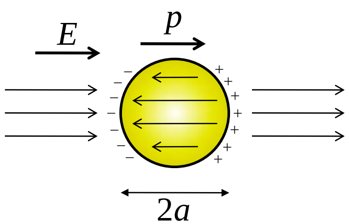
Propagating Plasmons
surface plasmon polariton (SPP)

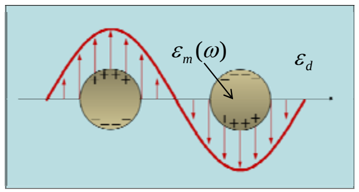




Localized surface plasmon resonance (LSPR)

- A metallic nanoparticle inside a electromagnetic field





  - dielectric functions: the metallic $\varepsilon_m(\omega)$ and of the dielectric host ε_d
  - in the electrostatic limit $a << \lambda$ the polarization is

$$p(\omega) \cong 4\pi a^3 \left(\frac{\varepsilon_m(\omega) - \varepsilon_d}{\varepsilon_m(\omega) + 2\varepsilon_d} \right) E(\omega)$$

- Resonance condition (LSPR) $\mathrm{Re}\{\varepsilon_m(\omega)\} = -2\varepsilon_d$

Nanoparticles in arrays

- Strong absorption and reflection at LSPR frequency
- An effective medium description
  - the Maxwell-Garnett effective medium

$$\frac{\tilde{\varepsilon}(\omega) - \varepsilon_d}{\tilde{\varepsilon}(\omega) + 2\varepsilon_d} = f \frac{\varepsilon_m(\omega) - \varepsilon_d}{\varepsilon_m(\omega) + 2\varepsilon_d}$$

  - NPs at spacing *L* have volume filling ratio *f*

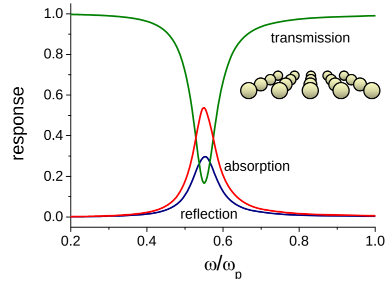
$$f = \frac{4\pi}{3} \frac{a^3}{L^3}$$

  - for a simple Drude for the metal

$$\varepsilon_m(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$

  - the effective medium for $\varepsilon_d = 1$

$$\tilde{\varepsilon}(\omega) = 1 + \frac{f\omega_p^2}{(1-f)\omega_p^2/3 - \omega^2 - i\gamma\omega}$$



effective medium is a Lorentz oscillator

- at eigenfrequency $\omega_p \sqrt{3(1-f)}$
- and decay rate γ
- NPs are like polarizable atoms

Realistic considerations

- The dielectric function is not a simple Drude model
  - get the actual one at "RefractiveIndex.info" (get index and change into dielectric function)
  - be careful of units, sometimes wavelength in microns, nanometers, eVs, etc…
- The host is usually not air
- The decay rate is increased due to scattering at the nanoparticle surface
  - surface scattering rate is $\gamma_{sc} = \upsilon_F / a$
  - total decay rate $\gamma' = \gamma + \gamma_{sc}$
  - the correction to the dielectric function

$$\varepsilon'_m(\omega) = \varepsilon_m(\omega) + \frac{\omega_p^2}{\omega^2 + i\gamma\omega} - \frac{\omega_p^2}{\omega^2 + i\gamma'\omega}$$

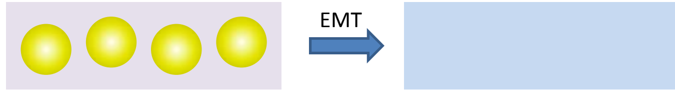
  - relevant numbers for Ag and Au

	ω_p [s^{-1}]	γ [s^{-1}]	υ_F [m/s^{-1}]
Ag	1.396E+16	2.536E+13	1.390E+06
Au	1.330E+16	1.033E+14	1.400E+06

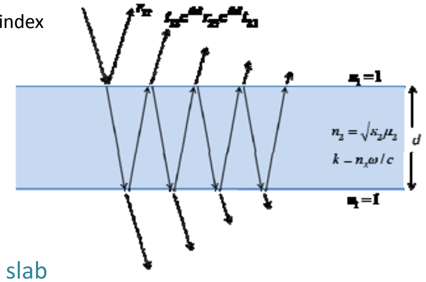
  - changing between units: $[eV] = [s^{-1}]/1.52\times10^{15}$ $\quad [nm] = 1240/[eV]$

Transmission through a slab

- Effective medium approach



  - n_2 is the effective index



- Reflectivity from a slab

$$R = \left| \frac{(n_2^2 - 1)\sin kd}{2n_2 \cos kd - i(n_2^2 + 1)\sin kd} \right|^2$$

Plasmonics lab exercise

- Explore the computational *vs* approximate analytical results for metallic spheres arranged in a square lattice:
  - effect of radius
  - effect of filling ratio
  - effect of periodicity
  - effect of host index
  - effect of metal content in core-shell
- Compare the calculated reflectance peak to the:
  - peak position of the polarizability in small particle limit
  - peak in the effective medium
  - peak in the reflectance from an effective medium
- Do the above for Ag or Au

Input file

```
0 1                                   :lateral size of box
4                                     :number of slabs
100 1.0                               :thickness and eps of slab
10  1.0                               :thickness and eps of slab
10  1.0                               :thickness and eps of slab
100 1.0                               :thickness and eps of slab
1                                     :number of objects
1 0 2                                 :(0/1/2 sp/cy/bl),(0/1 sq/hx),Layer
20 20 10 10 10 -400.0105 2 1 1:Lx, Ly, Sx, Sy, Sz, eps
0 0 0                                 :positioning parameters
0  0  0  0  0  0                      :positioning parameters
100 100                               :lattice parameters
450 450 300 800 200                   :source parameters
0 1 0                                 :source parameters
0 0 5 0 0 1                           :source parameters
1                                     :number of different materials
1 1                                   :material: 1=Ag, 2=Au
0                                     :calculation parameters
0                                     :calculation parameters
0                                     :calculation parameters
```