DPMS: Advanced Materials

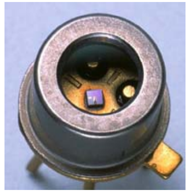
Lecture Y4:
Computational Optics I

Elefterios Lidorikis
Room Π1, 26510 07146
elidorik@cc.uoi.gr
http://cmsl.materials.uoi.gr/lidorikis

Photonic and optoelectronic technologies

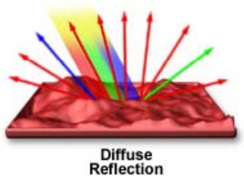
- Understanding light-matter interactions is crucial for new applications

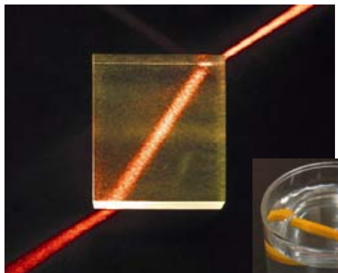


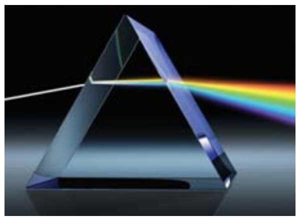



Reflection and refraction

- Material property:
  - dielectric function
  - index of refraction

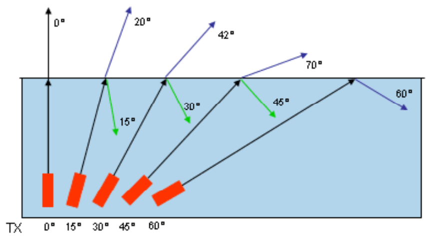


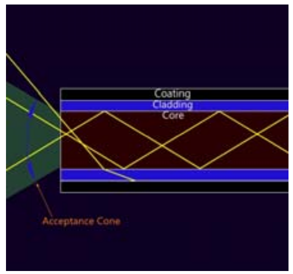


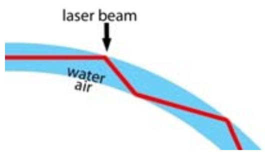


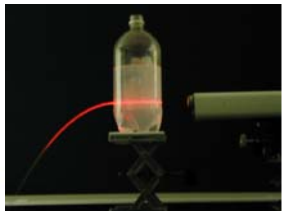
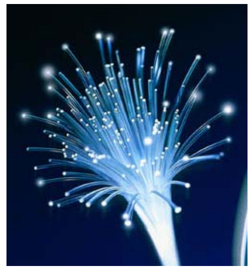
Trapping and guiding light

- Total internal reflection



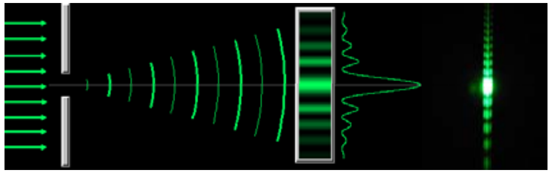
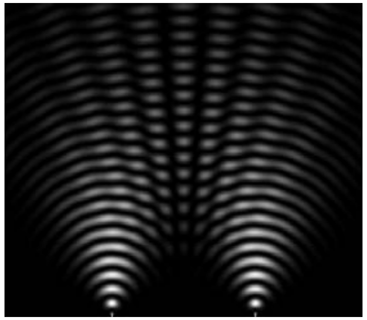
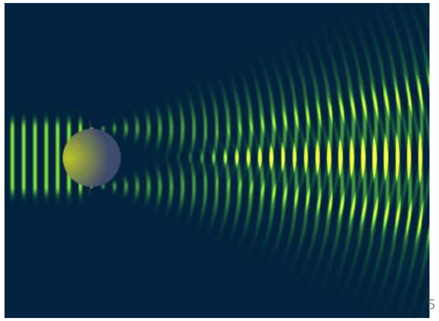




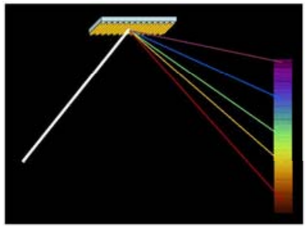
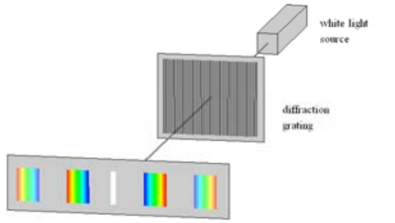
Diffraction and interference

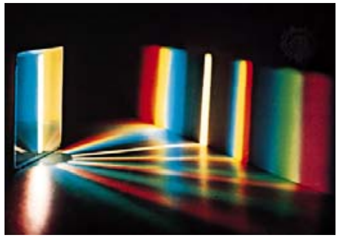
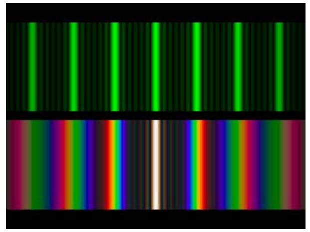
- Diffracted waves interfere

Diffraction gratings

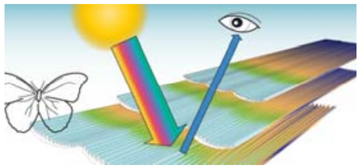
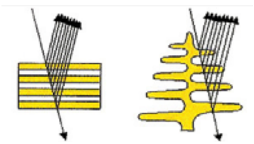
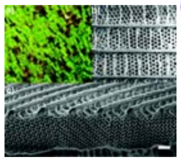
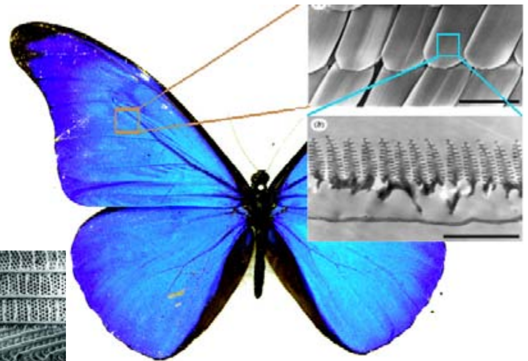
- Diffraction gratings are used for wavelength separation

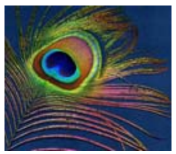




Structural color

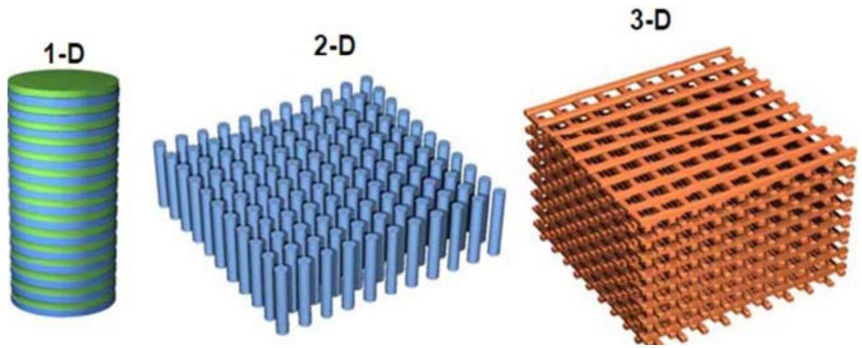
- Natures diffraction gratings
  - photonic crystals

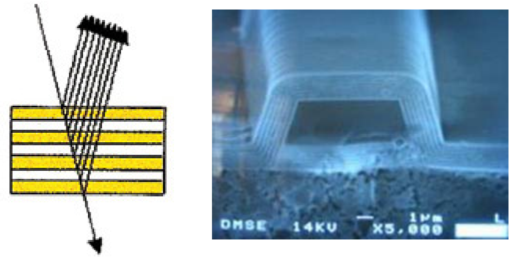


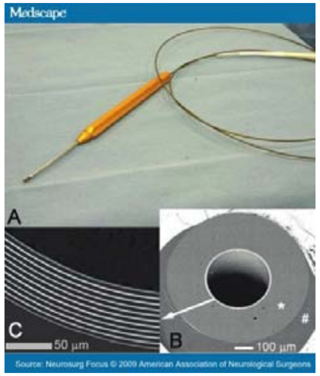
Photonic crystals in technology

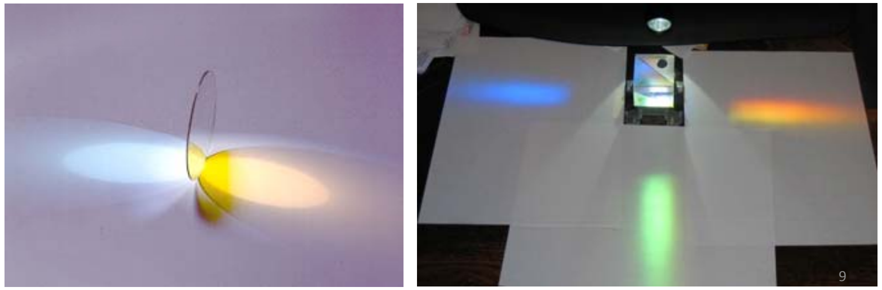
- Applications in extreme light manipulation



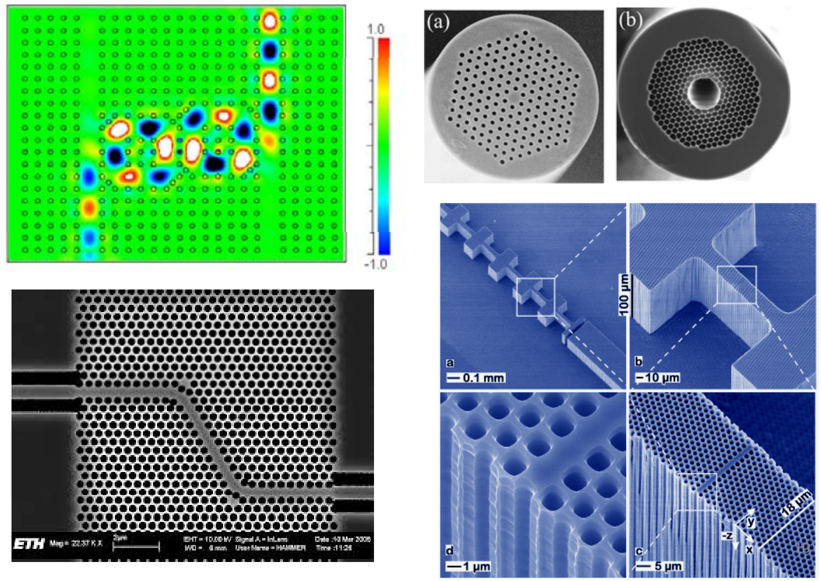
Examples of 1D photonic crystals



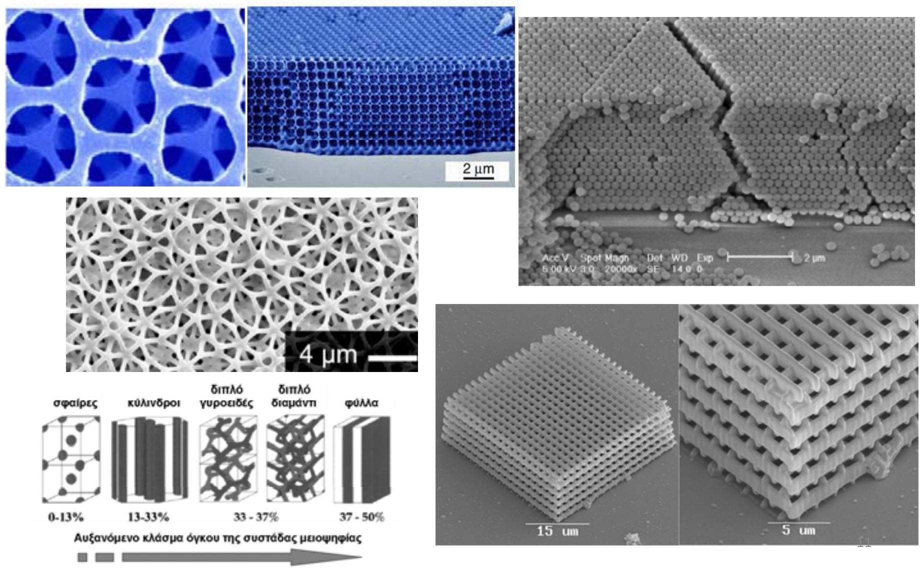




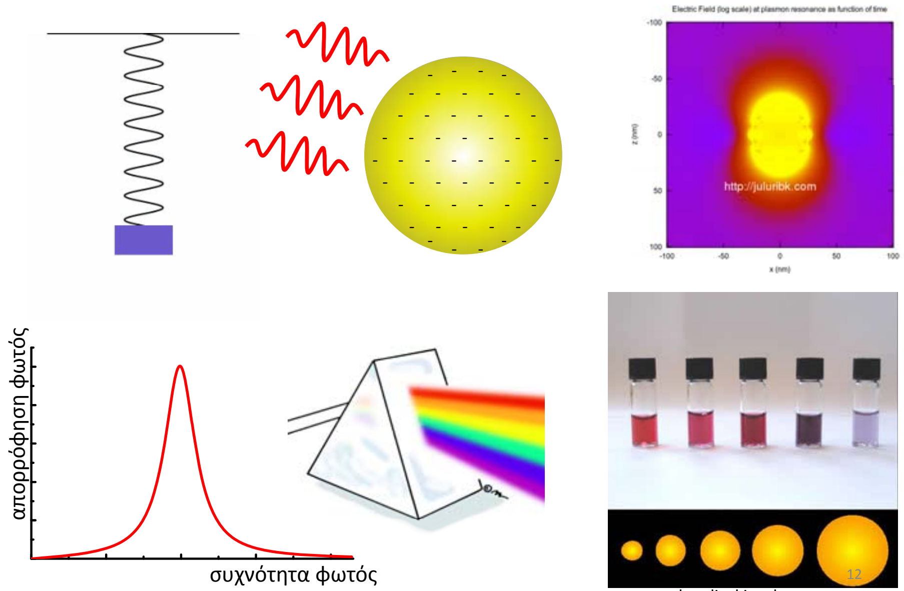
Examples of 2D photonic crystals



Examples of 3D photonic crystals

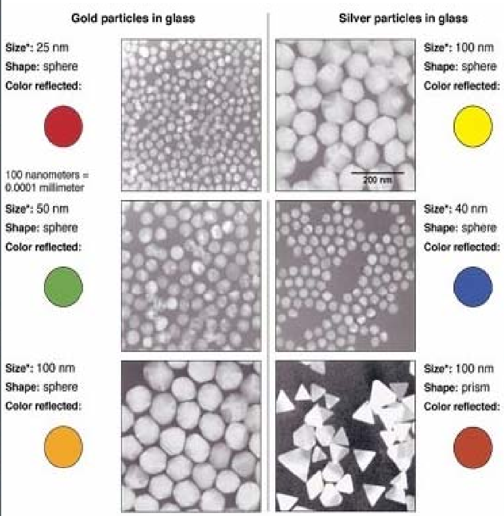


Plasmonics: interactions with nanostructured metals



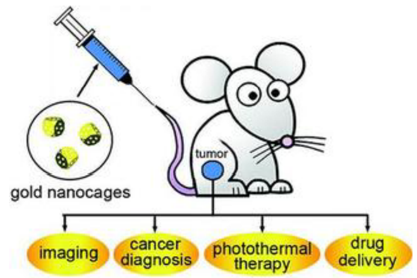
kondinski.webs.com

Plasmonics in the middle ages

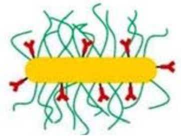


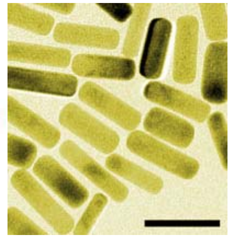
Institute of Nanotechnology, Northwestern University

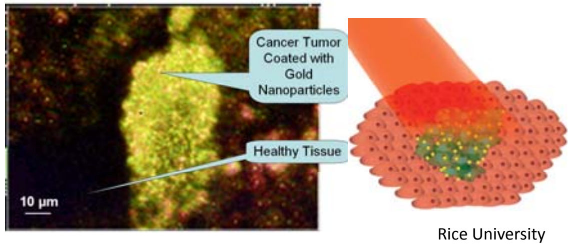
Εφαρμογές πλασμονικών νανοσωματιδίων στην ιατρική



anti-EGFR conjugated gold nanoparticles

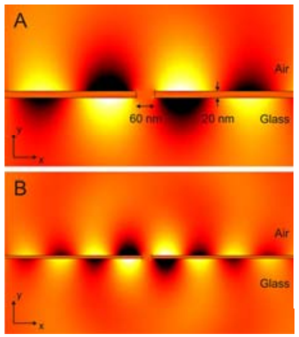


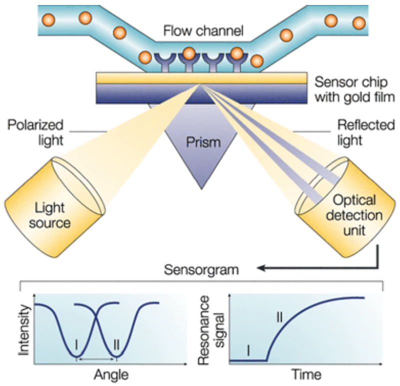


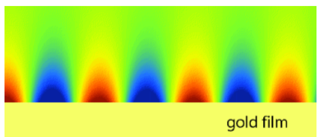


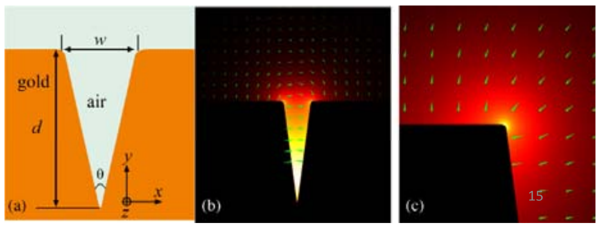
Rice University

Surface plasmons







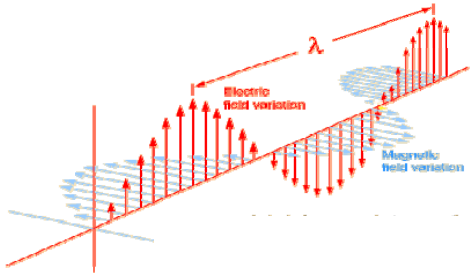


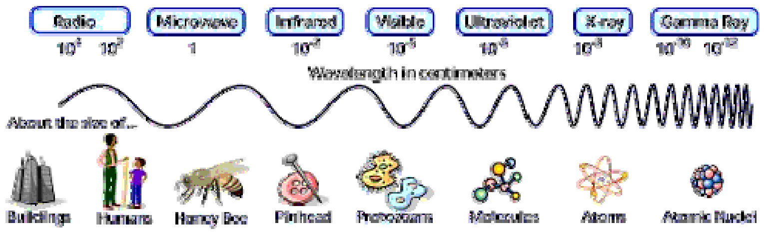
Outline

- E/M waves
- Wave equations
- Boundary conditions
- Materials’ optical response
- Materials’ optical characterization
- Numerical solutions
- Applications design

The classical nature of light

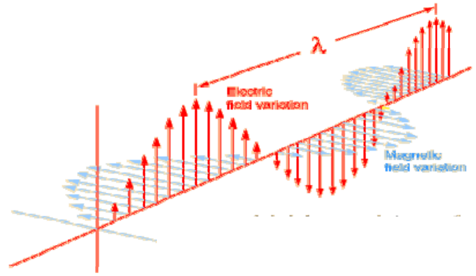
- Oscillating electric and magnetic fields
  - propagation speed $c=3\times10^8$ m/s
- Transverse waves
  - perpendicular to propagation direction
  - perpendicular to each other
- Gets polarized
  - linearly polarized (e.g. x and y)
  - circularly polarized (e.g. right and left)
  - generally two orthogonal polarizations
- Interaction with materials
  - reflection, refraction, absorption, interference, scattering, diffraction, …





E/M wave properties

- Wavelength λ
  - spatial periodicity
- Period T
  - temporal periodicity
- Wavevector $k=2\pi/\lambda$
  - spatial repetition rate
- Angular frequency $\omega=2\pi/T$
  - temporal repetition rate
- Dispersion relation $k=n\omega/c$ (n is index of refraction)
  - relation between k and ω
  - relation between space and time
  - relation between momentum and energy ($E=\hbar\omega,\ \ p=\hbar k$)
- In 3D space, **k** is a 3D vector
- Electric and magnetic fields are 3D vectors
  - polarization of wave is the electric field polarization



E/M wave equations

- Maxwell's equations

$$\nabla\cdot\mathbf{D}=0 \qquad \nabla\cdot\mathbf{B}=0 \qquad \nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t} \qquad \nabla\times\mathbf{H}=+\frac{\partial\mathbf{D}}{\partial t}$$

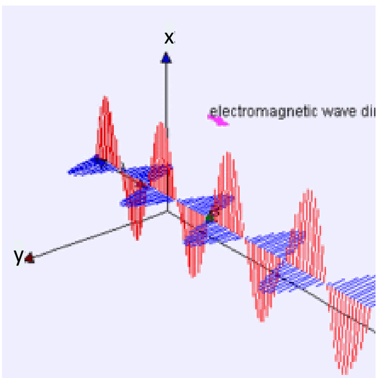
$$\mathbf{D}\equiv\mathbf{D}(\mathbf{r},t) \qquad \mathbf{B}\equiv\mathbf{B}(\mathbf{r},t) \qquad \mathbf{E}\equiv\mathbf{E}(\mathbf{r},t) \qquad \mathbf{H}\equiv\mathbf{H}(\mathbf{r},t)$$

- Constitutive relations

$$\mathbf{D}=\varepsilon_0\mathbf{E}+\mathbf{P}=\varepsilon_0\varepsilon_r\mathbf{E}=\varepsilon\cdot\mathbf{E}$$

$$\mathbf{B}=\mu_0(\mathbf{H}+\mathbf{M})=\mu_0\mu_r\mathbf{H}=\mu\cdot\mathbf{H}$$

- Material properties
  - electric permittivity $\varepsilon\equiv\varepsilon(\mathbf{r})$
  - magnetic permeability $\mu\equiv\mu(\mathbf{r})$
  - refractive index $n=n(\mathbf{r})=\sqrt{\varepsilon_r(\mathbf{r})\mu_r(\mathbf{r})}$
- At optical frequencies $\mu_r=1$



E/M wave equations in 1D

- Maxwell's equations

$$\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t} \ \overset{\text{1D}}{\Rightarrow}\ \frac{\partial E}{\partial z}=-\mu_0\frac{\partial H}{\partial t}$$

$$\nabla\times\mathbf{H}=+\frac{\partial\mathbf{D}}{\partial t} \ \Rightarrow\ -\frac{\partial H}{\partial z}=\varepsilon_0\varepsilon_r\frac{\partial E}{\partial t}$$

- Combine for one unique equation

$$\frac{\partial E}{\partial z}+\mu_0\frac{\partial H}{\partial t}=0 \quad \Rightarrow\frac{\partial}{\partial z}\left(\frac{\partial E}{\partial z}+\mu_0\frac{\partial H}{\partial t}\right)=0$$

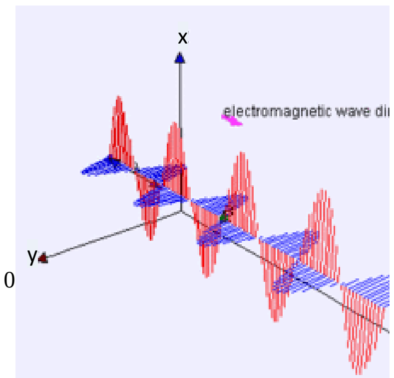
$$\Rightarrow\frac{\partial^2 E}{\partial z^2}+\mu_0\frac{\partial}{\partial t}\frac{\partial H}{\partial z}=0 \quad \Rightarrow\frac{\partial^2 E}{\partial z^2}-\varepsilon_0\mu_0\varepsilon_r\frac{\partial}{\partial t}\frac{\partial E}{\partial t}=0$$

$$\Rightarrow\frac{\partial^2 E}{\partial z^2}-\frac{\varepsilon_r}{c^2}\frac{\partial^2 E}{\partial t^2}=0 \qquad c^2=1/(\varepsilon_0\mu_0)$$

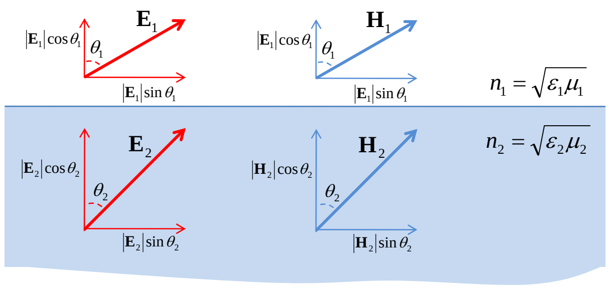
- Wave solution are plane waves

$$\mathbf{E}=\hat{x}E_0\mathrm{e}^{i(kz-\omega t)}$$

  - dispersion relation $-k^2E_0\mathrm{e}^{i(kz-\omega t)}+\frac{\varepsilon_r\omega^2}{c^2}E_0\mathrm{e}^{i(kz-\omega t)}=0 \quad\Rightarrow k=\sqrt{\varepsilon_r}\,\omega/c=n\omega/c$



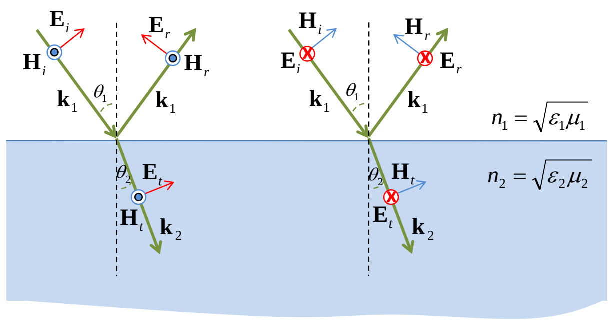
Boundary conditions at interfaces



- Continuity at the boundary:
  - of the parallel components of the electric field $\mathbf{E}_{//}$ $\quad |\mathbf{E}_1|\sin\theta_1 = |\mathbf{E}_2|\sin\theta_2$
  - of the perpendicular components of the displacement $\mathbf{D}_\perp$ $\quad \varepsilon_1|\mathbf{E}_1|\cos\theta_1 = \varepsilon_2|\mathbf{E}_2|\cos\theta_2$
  - of the parallel components of the magnetic field $\mathbf{H}_{//}$ $\quad |\mathbf{H}_1|\sin\theta_1 = |\mathbf{H}_2|\sin\theta_2$
  - of the perpendicular components of the inductance $\mathbf{B}_\perp$ $\quad \mu_1|\mathbf{H}_1|\cos\theta_1 = \mu_2|\mathbf{H}_2|\cos\theta_2$

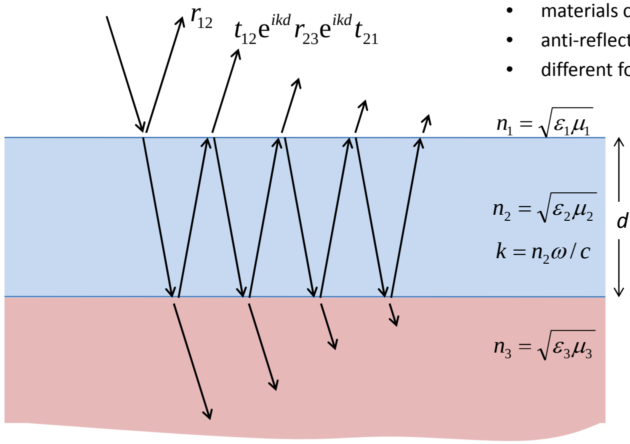
Reflection and refraction at an interface

transverse magnetic (TM) *p-polarization* — *transverse electric (TE)* *s-polarization*



- Boundary conditions on **k**
  - parallel component of **k** conserved $\quad |\mathbf{k}_1|\sin\theta_1 = |\mathbf{k}_2|\sin\theta_2 \qquad |\mathbf{k}| \equiv k = n\omega/c$
  - momentum conservation $\quad n_1\sin\theta_1 = n_2\sin\theta_2$ Snell's law
- Boundary conditions on fields
  - reflection and transmission amplitudes $\quad r_{12},\ t_{12}$
  - reflectivity and transmittance $\quad R = |r_{12}|^2,\quad T = (n_2/n_1)|t_{12}|^2$
- Inside materials $\quad \lambda = \lambda_0/n,\quad \upsilon = c/n$

Reflection and transmission from a thin film



- materials characterization
- anti-reflection coatings
- different for *s* and *p* polarizations

at normal incidence

$$r_{ij} = \frac{n_i - n_j}{n_i + n_j}$$

$$t_{ij} = \frac{2n_i}{n_i + n_j}$$

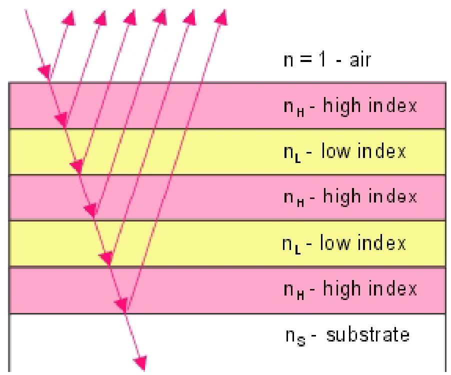
- Total reflection

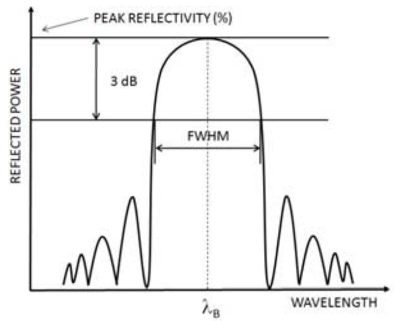
$$r = r_{12} + t_{12}e^{ikd}r_{23}e^{ikd}t_{21} + t_{12}e^{ikd}r_{23}e^{ikd}r_{21}e^{ikd}r_{23}e^{ikd}t_{12} + \ldots$$

$$= r_{12} + t_{12}r_{23}t_{21}e^{i2kd}\cdot[1 + r_{21}r_{23}e^{i2kd} + (r_{21}r_{23}e^{i2kd})^2 + \ldots] \quad = r_{12} + \frac{t_{12}r_{23}t_{21}e^{i2kd}}{1 - r_{21}r_{23}e^{i2kd}}$$

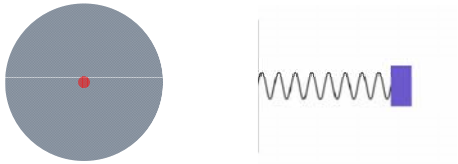
Reflection from periodic film arrays

- 1D photonic crystal – Bragg mirror
  - multiple reflections result into extreme reflection for some frequencies
  - perfect mirrors for lasers, selective filters, sensors, etc





Dielectric function: material polarizability



- Driven oscillation $m\frac{d^2r}{dt^2} = -m\gamma\frac{dr}{dt} - Kr - eE$ $\quad \omega_0 = \sqrt{K/m} \Rightarrow K = m\omega_0^2$
- Assume harmonic oscillation $r = r_0 e^{-i\omega t}$ $\quad E = E_0 e^{-i\omega t}$

$$-\omega^2 mr = i\omega m\gamma r - m\omega_0^2 r - eE \quad \Rightarrow r = -\frac{eE}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

- Polarization depends on number density of electronic orbitals

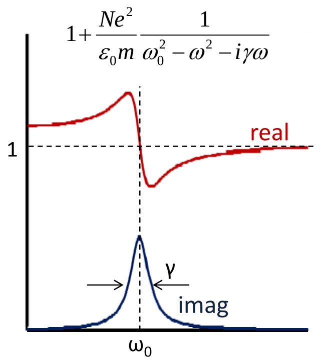
$$P = -Ner = \frac{Ne^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}E \qquad D = \varepsilon_0\varepsilon_r E = \varepsilon_0 E + P = \varepsilon_0\left(1 + \frac{Ne^2}{\varepsilon_0 m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}\right)E$$

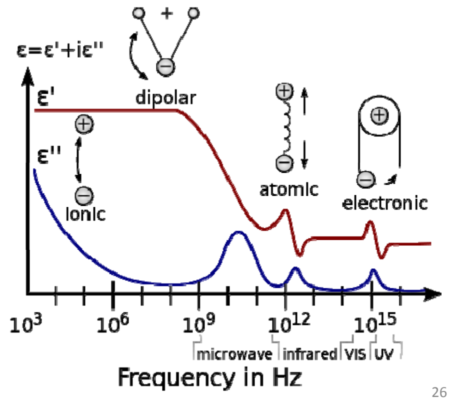
- Dielectric function $\varepsilon_r = 1 + \frac{Ne^2}{\varepsilon_0 m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$

Dielectric function

- Each orbital has a different contribution
  - electronic: UV and Visible
  - atomic: IR
  - etc

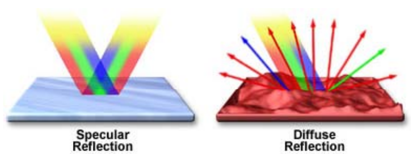
$$\varepsilon_r = 1 + \sum_i \frac{N_i e^2}{\varepsilon_0 m_i}\frac{1}{\omega_{0i}^2 - \omega^2 - i\gamma_i\omega}$$



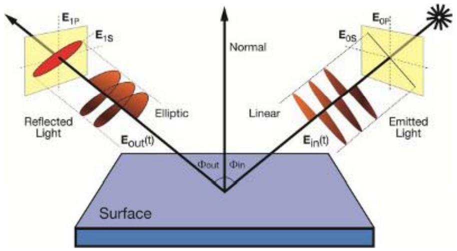


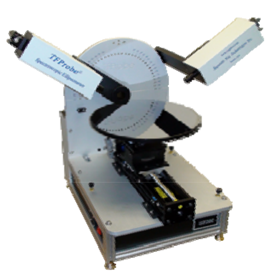
Materials' optical characterization

- Reflectance spectroscopy



- Ellipsometry





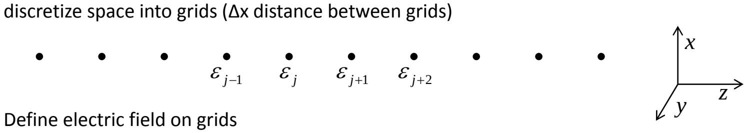
Numerical solution

- Consider 1D Maxwell's equations

$$\frac{\partial E_x}{\partial z} = -\mu_0\frac{\partial H_y}{\partial t}, \qquad \frac{\partial H_y}{\partial z} = -\varepsilon\frac{\partial E_x}{\partial t}$$

- Finite-difference time-domain method (FDTD)
  - discretize space into grids (Δx distance between grids)

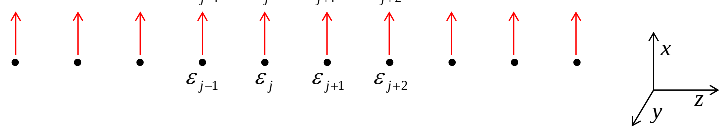
$\varepsilon_{j-1} \quad \varepsilon_j \quad \varepsilon_{j+1} \quad \varepsilon_{j+2}$



  - Define electric field on grids

$E_{j-1}^n \quad E_j^n \quad E_{j+1}^n \quad E_{j+2}^n$

$\varepsilon_{j-1} \quad \varepsilon_j \quad \varepsilon_{j+1} \quad \varepsilon_{j+2}$



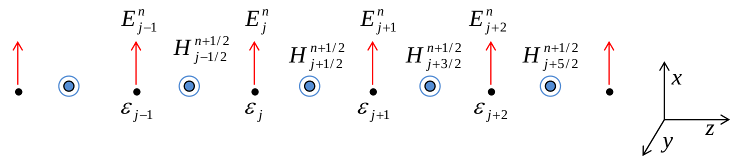
  - we will also discretize time into time-steps (Δt time between time-steps)

$E_j^{n-1} \quad E_j^n \quad E_j^{n+1} \quad E_j^{n+2}$

  - put magnetic field at half grids and half time-steps $H_{j-1/2}^{n+1/2} \quad H_{j+1/2}^{n+1/2} \quad H_{j+3/2}^{n+1/2}$

1D FDTD

- Space-time grid



- Approximate Maxwell's equations by central differences
  - Assume we know everything for E at time n-1 and for H at time n-1/2

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon}\frac{\partial H_y}{\partial z} \quad \to \frac{E^n_j - E^{n-1}_j}{\Delta t} = -\frac{1}{\varepsilon_j}\frac{H^{n-1/2}_{j+1/2} - H^{n-1/2}_{j-1/2}}{\Delta z}$$

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0}\frac{\partial E_x}{\partial z} \quad \to \frac{H^{n+1/2}_{j+1/2} - H^{n-1/2}_{j+1/2}}{\Delta t} = -\frac{1}{\mu_0}\frac{E^n_{j+1} - E^n_{j-1}}{\Delta z}$$

- Field update algorithm

$$E^n_j = E^{n-1}_j - \frac{c\Delta t}{\Delta z}\frac{1}{\varepsilon_j}\left(H^{n-1/2}_{j+1/2} - H^{n-1/2}_{j-1/2}\right)$$

$$H^{n+1/2}_{j+1/2} = H^{n-1/2}_{j+1/2} - \frac{c\Delta t}{\Delta z}\left(E^n_{j+1} - E^n_{j-1}\right)$$

the normalization was made

$$E \to \sqrt{\varepsilon_0 / \mu_0}\, E$$

1D stability condition

$$c\Delta t < \Delta z$$

2D and 3D FDTD

- Yee lattice: different sublattices for electric and magnetic fields
  - central differences for all field components