Optical spectroscopy and biosensors for investigation of biomolecules and their interactions

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Fundamentals of Optics for Probing and Manipulation with Matter

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Content

- **Light propagation description (rays, waves, polarization)**
- **Total internal reflection (TIR)**
- **Optical guided waves**
- **Definition of refractive index**
- **Effective medium theory, absorbing media.**
- **Examples of interaction of light with matter and light – matter manipulation, optical tweezers, surface plasmons….**

Optics / Photonics - Light Propagation / Confinement

Propagation of light and its interaction with matter can be treated at different levels (accuracy):

Less accurate (and simpler to use…)

		Size of an object Δx
Ray optics	- refraction, reflection…	$\Delta x >> \lambda$
Wave optics	- wavelength λ, phase, interference…	$\Delta x <\sim \lambda$
Electromagnetic optics	- polarization, surface waves…	
Quantum optics	- quantized energies (photons), lasers…	

More general (and complicated…)

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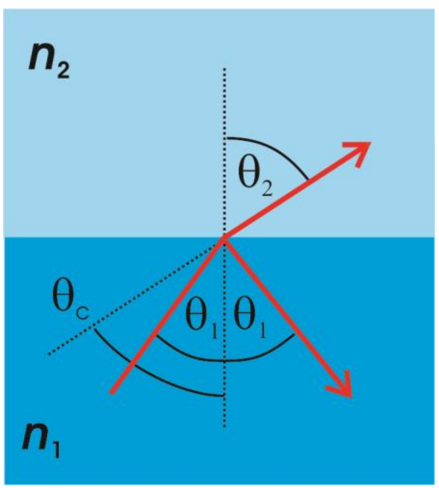
Ray Optics

Refractive index *n* describes optical density of matter in which a light beam – ray – propagates. At a plane interface between $n_1 > n_2$, reflection and refraction occurs.

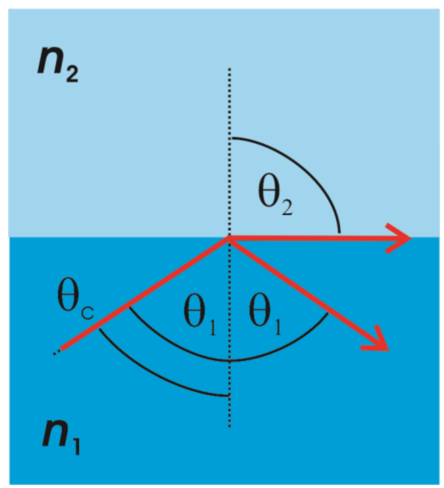
Snell law $$n_1 \sin(\theta_1) = n_2 \sin(\theta_2) \Rightarrow \theta_c = \arcsin(n_2 / n_1)$$

$\theta_1 < \theta_c$



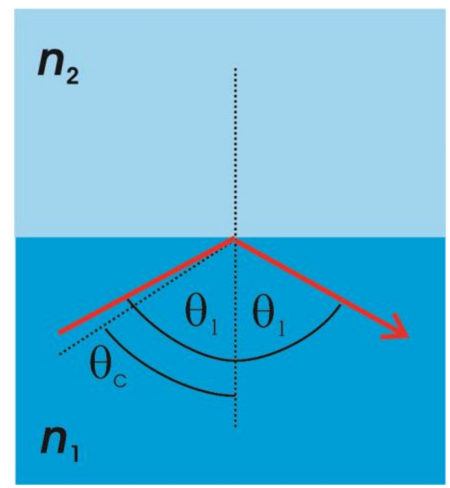
Refracted beam propagates to n_2 medium

$\theta_1 = \theta_c$



Beam propagates along the interface

$\theta_1 > \theta_c$



Beam undergoes total internal reflection - TIR

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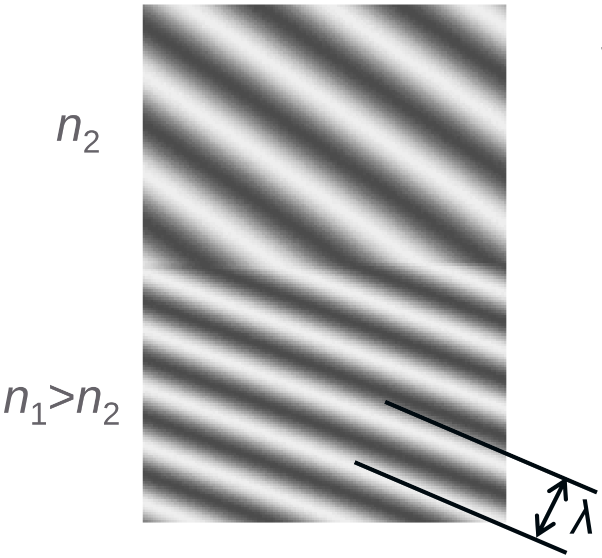
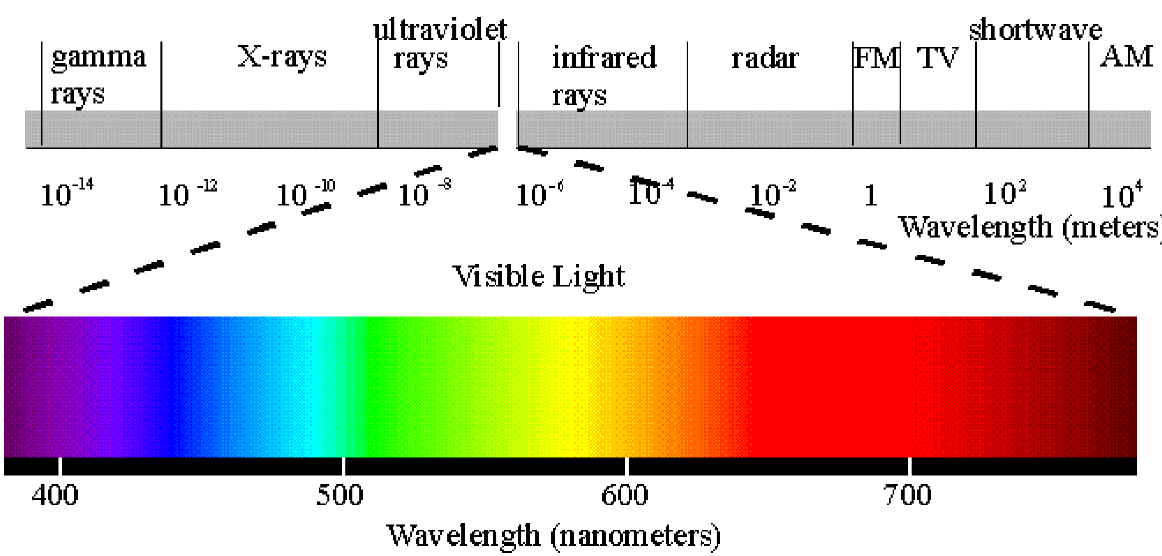
Wave Optics



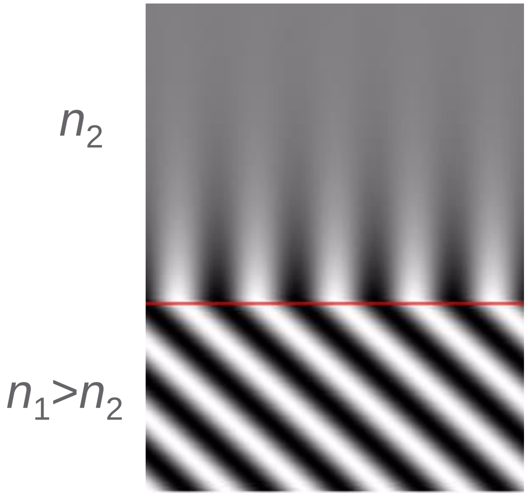
Wave equation $$\left(\frac{d^2}{dx^2}-\frac{1}{v^2}\frac{d^2}{dt^2}\right)u(x,t)=0$$

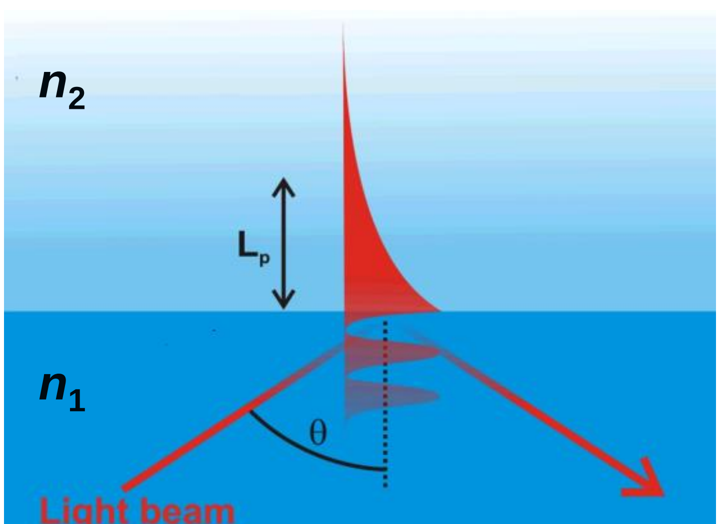
Plane wave (scalar) $$u(x,t)=A\sin(k_0 n x-\omega t)$$

$k_0=\omega/c$	propagation constant in vacuum
ω	angular frequency
$v=c/n$	velocity of light
$\lambda=2\pi c/\omega$	wavelength in vacuum



Total Internal Reflection - TIR





At angles $\theta > \theta_c$ field amplitude exponentially decays to medium n_2

$$u(x) = u_0 e^{-x/L_p}$$

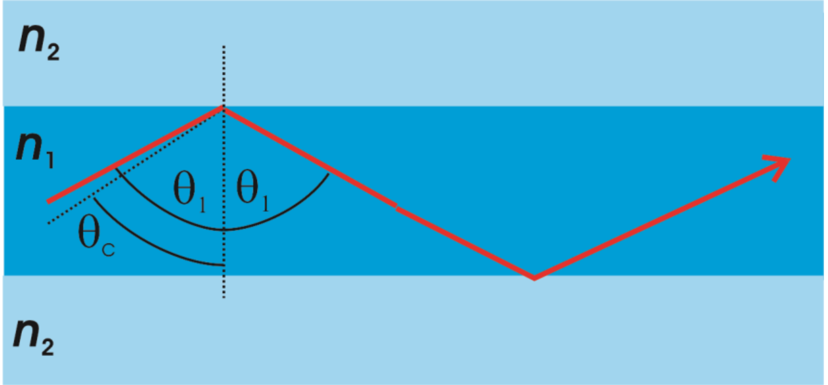
The field probes limited penetration depth from the interface:

$$L_p = \frac{\lambda}{4\pi\sqrt{n_1^2 \sin^2(\theta) - n_2^2}}$$

Slab Optical Waveguide

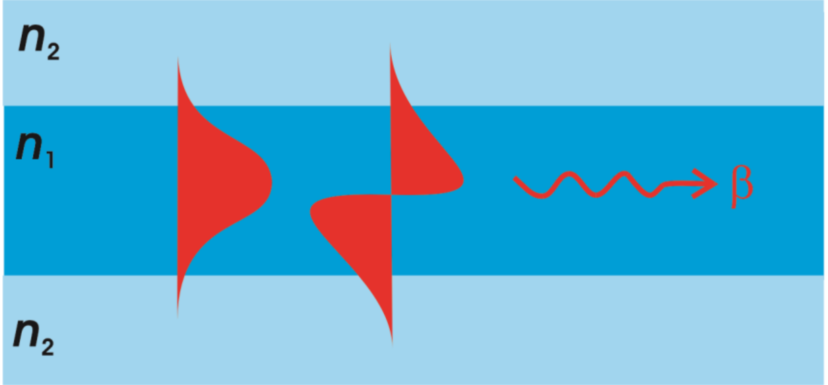
Ray optics point of view:

Light propagation is confined by TIR at opposite interfaces

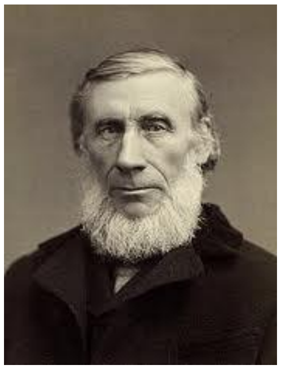


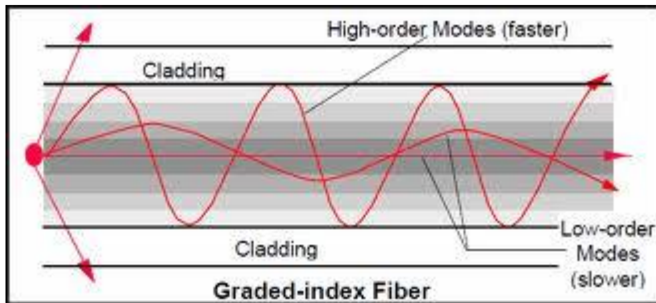
Wave optics point of view:

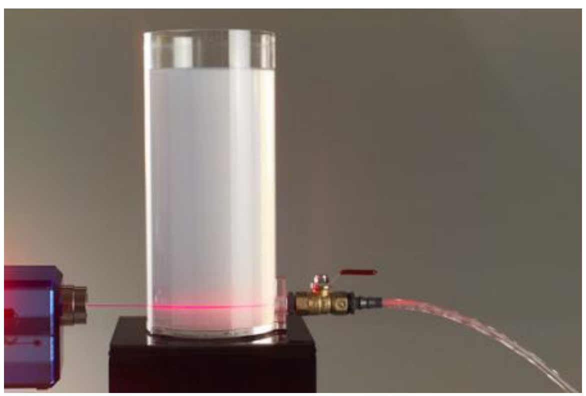
Only discrete modes with certain propagation constants β can travel through the waveguide

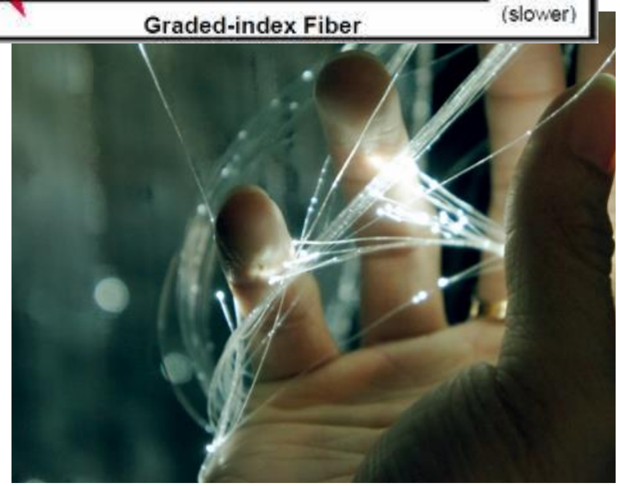


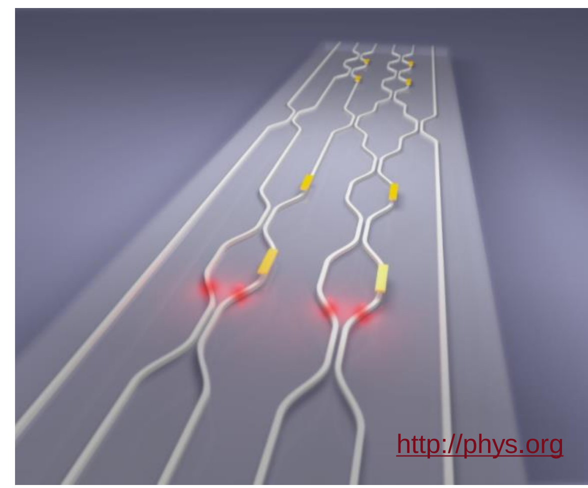
Examples of Dielectric Optical Waveguide











http://phys.org

Historical Tyndall experiment at 1870.

Optical fibers

Optical circuits

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Examples of Dielectric Optical Waveguide

Optical fiber bundles used for imaging of remote places (right) and catheters (down).

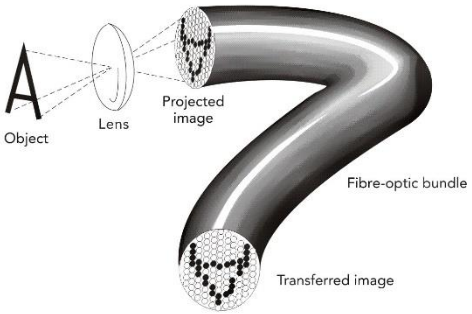
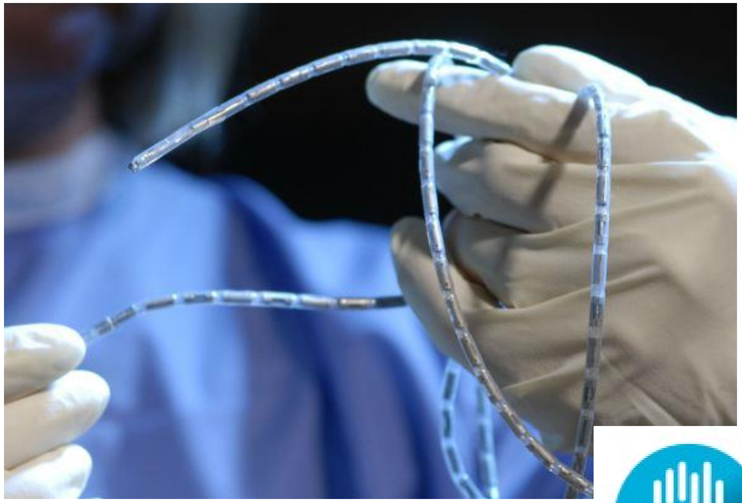


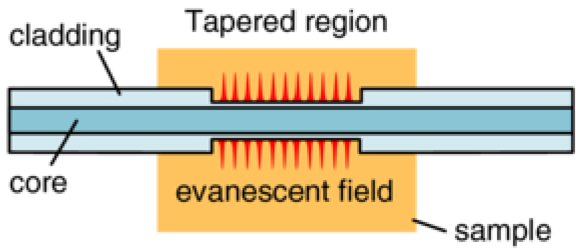
Figure 7-4 Fiber optic endoscopy



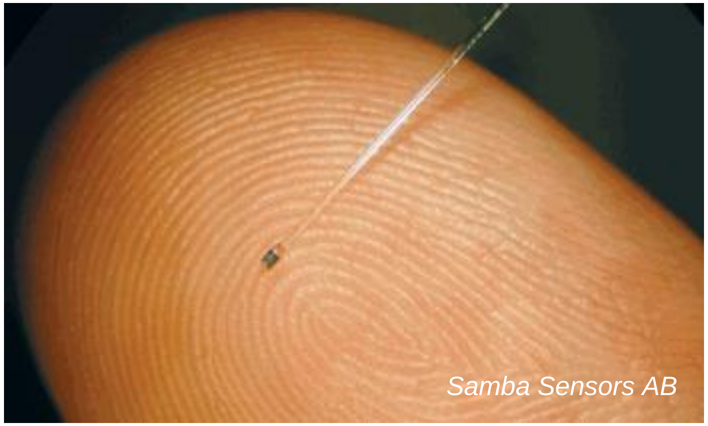
CSIRO

Examples of Dielectric Optical Waveguide

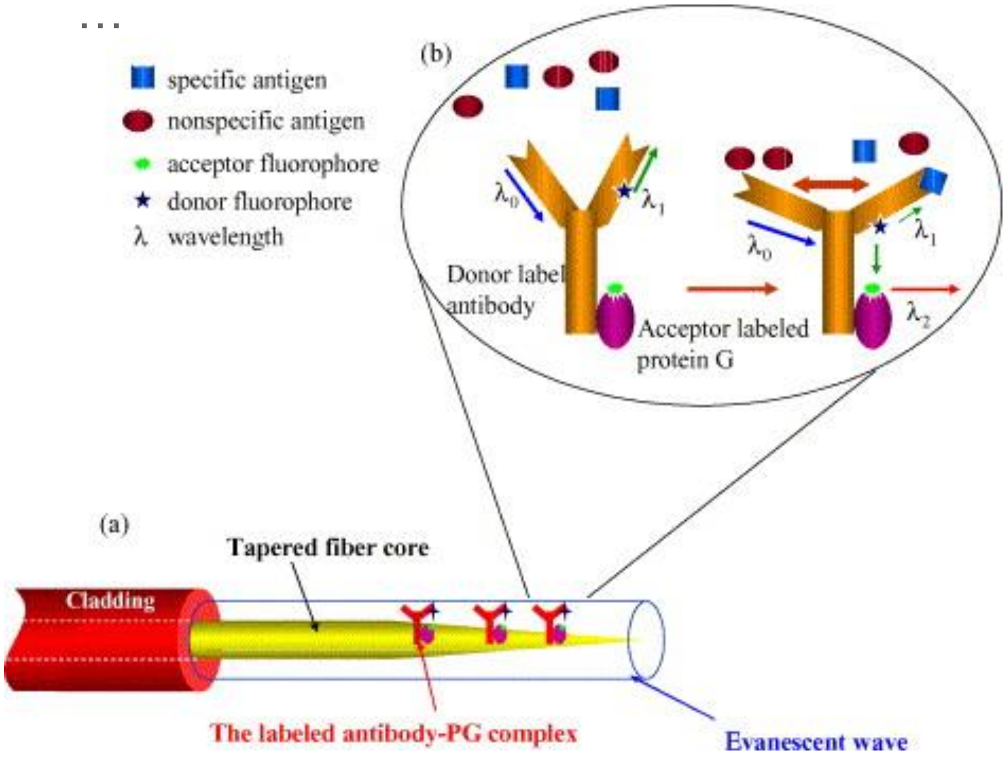
Optical fibers allow for design of miniature sensors relying on probing by evanescent field:



Hodgkinson et al, 2013 *Meas. Sci. Technol.* **24** 012004



Oxygen
Pressure
Fluorescence, FRET
…



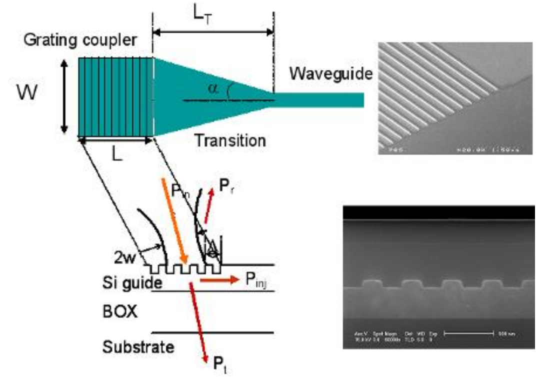
Sungho Biosensors and Bioelectronics
Volume 21, Issue 7, 15 January 2006, Pages 1283–1290

Coupling of Light to Dielectric Optical Waveguides

Directly incident light on a waveguide does not excited guided waves as a phase-matching condition needs to be fulfilled. A means to enhance the momentum (wave-vector) of the light needs to be used:

Grating coupler

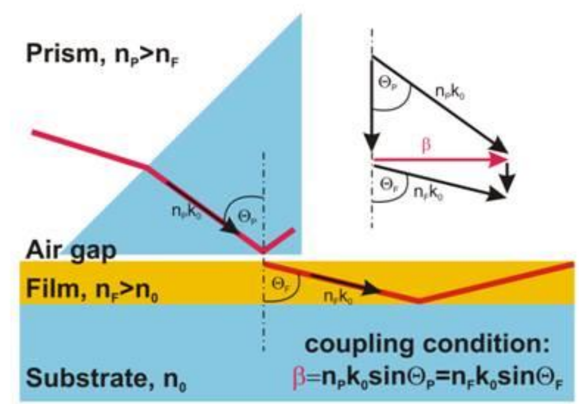
$$\beta = k_0 n \sin(\theta) + p\frac{2\pi}{\Lambda}$$



http://silicon-photonics.ief.u-psud.fr

Prism coupler

$$\beta = k_0 n_p \sin(\theta)$$



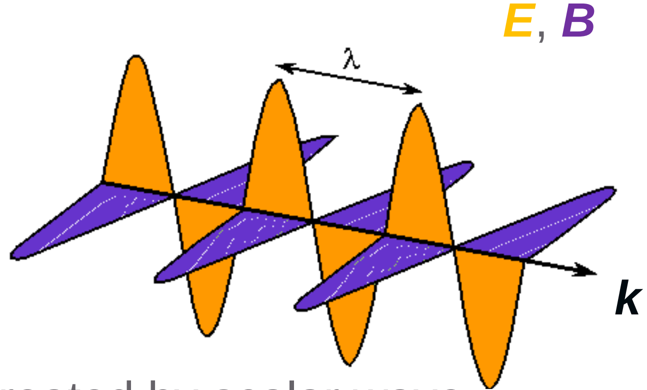
http://www.sciner.com

Electromagnetic Optics

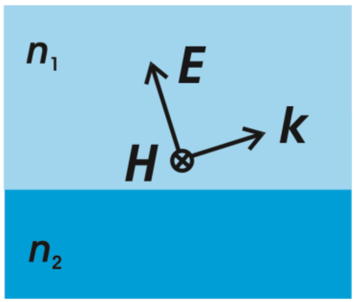
Describes light as a vector field with electric *E* and magnetic *B* components. Polarization (orientation of *E* and *B* vectors) is important in additional phenomena (e.g. surface plasmon resonance - SPR). Solution can be determined by set of Maxwell equations and boundary conditions:

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

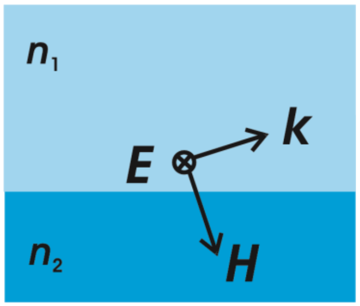
$$\nabla . \vec{D} = \rho \qquad \nabla . \vec{B} = 0$$



For planar interfaces, two set of solution can be treated by scalar wave equation:

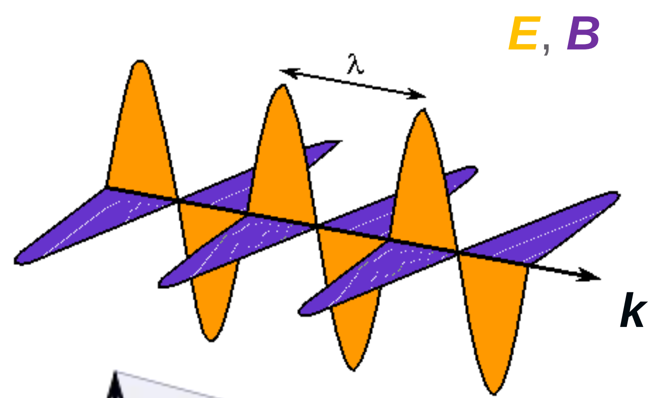


Transverse magnetic (TM, p)

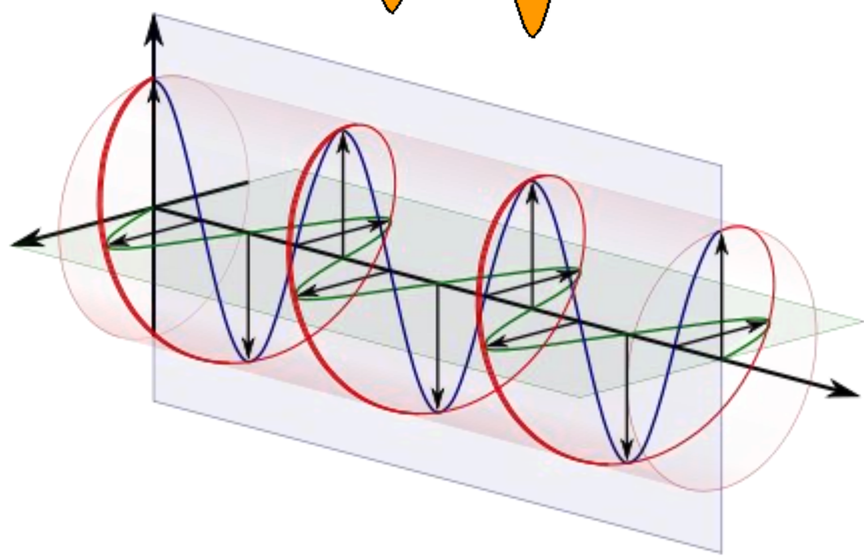


Transverse electric (TE, s)

Electromagnetic Optics
Polarization



Linear polarization:



Circular polarization:
can be described as a combination of two phase shifted linear polarizations.

'Maxwell‘s Macroscopic Equations'

The interaction of EM waves with matter is introduced through the permittivity ε and permeability μ. Attributed to space filled with atoms / molecules… and averaged over their ensemble (thus macroscopic, size << λ and >> then distance between atoms).

$\vec{E}$ Electric field

$\vec{B}$ Magnetic vector

$\vec{D} = \varepsilon_0 \vec{E} + \vec{P}$ Displacement field

$\vec{H} = \dfrac{\vec{B}}{\mu_0} - \vec{M}$ Magnetizing field

$\vec{j}$ Current density

ρ Charge density

$\vec{P}$ Polarizability

$\vec{M}$ Magnetization

$c = \dfrac{1}{\sqrt{\varepsilon_0 \mu_0}}$ Light velocity in vacuum

Dielectric Materials

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon_0 \vec{E}(1+\chi) = \varepsilon_0 \varepsilon \vec{E}$$

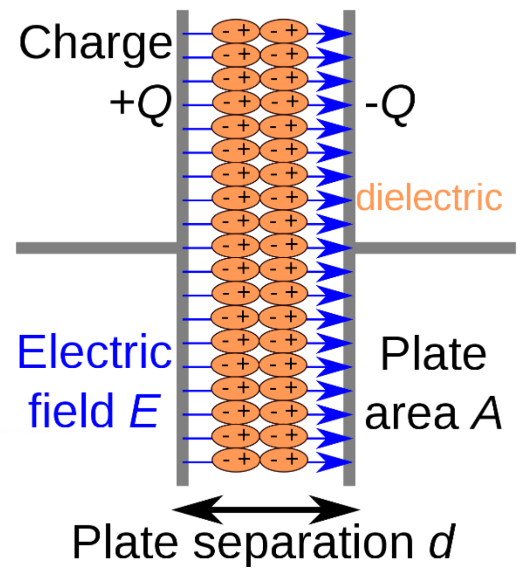
χ Susceptibility

For more details, see Lorenz Lorenz or Clausius-Mossotti theories for taking the local and macroscopic field into account:

$$\frac{\chi}{(3+\chi)} = \frac{N\alpha}{3\varepsilon_0}$$

α Polarizability

$$\boxed{n^2 = \varepsilon \qquad \text{Refractive index}}$$



$$n^2 + 2 = \frac{3}{1 - \frac{4}{3}\pi \frac{N_A}{M_w}\rho\alpha}$$

n – Refractive Index
N_A – Avogadro's constant
M_w – Molar weight
ρ – Density
α – Molecular polarizability

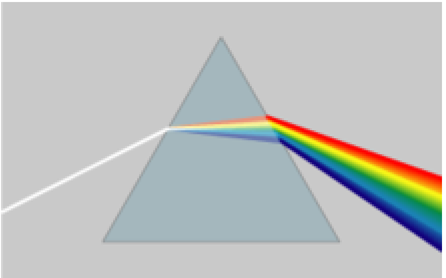
Yang; C., Jenekhe, S. *Chem. Mater.* 1995, *7*, 1276

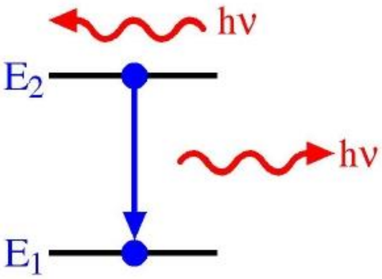
Complex Refractive Index

Parameter that describes interaction of light with matter composed of elements (e.g. atoms) that are << λ and exhibit polarizability. By averaging over many atoms that are be polarized by the oscillating electric field.

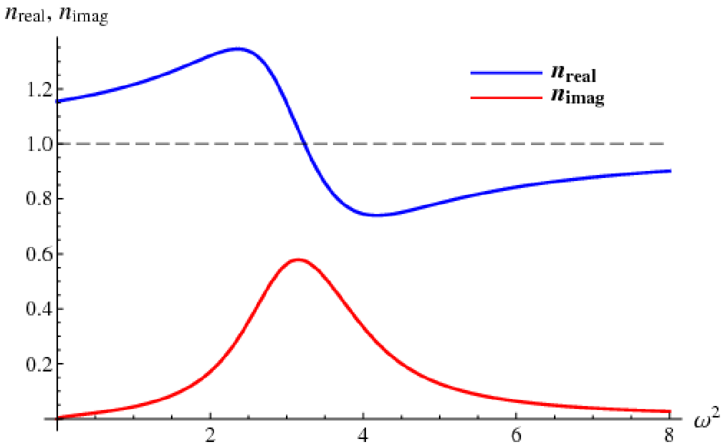
$$\tilde{n} = n + ik$$

Real part – refraction





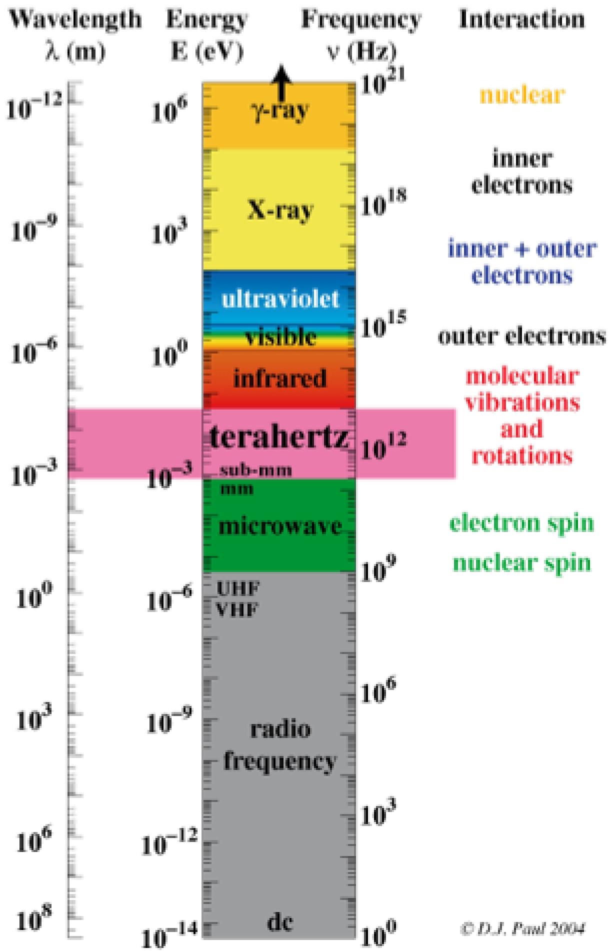
Imaginary part - absorption



Kramers-Kronig relations

Absorption of Molecules

Absorption of light by molecules is accompanied with their transition from a ground state to excited state (followed by a relaxation). It typically occurs at distinct energies leading to specific bands in absorption spectrum:



<u>Electronic lines</u> correspond to a change in the electronic state of an atom or molecule. Typically UV-Vis.

<u>Vibrational lines</u> correspond to changes in the vibrational state of the molecule and are typically found in the infrared region.

<u>Rotational lines</u>, for instance, occur when the rotational state of a molecule is changed. Rotational lines are typically found in the microwave spectral region.

Combination of above can lead to rather complex spectra.

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Complex Refractive Index

Often electric field is described by using complex numbers, reason is that mathematically some operations can be performed easier. However, physical meaning has only the real (or imaginary) part of it.

$$\vec{E} = \mathrm{Re}\left\{ \vec{E}_0 e^{-i\left(\omega t - \frac{2\pi}{\lambda}[n+ik]x\right)} \right\} = \vec{E}_0 \sin\left(\omega t - \frac{2\pi}{\lambda} n x\right) e^{-\frac{2\pi}{\lambda} k x}$$

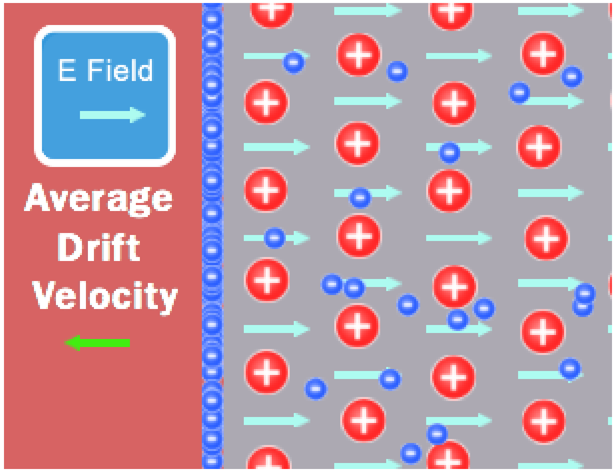
Wave behavior (as discussed for scalar field)

Exponential decay, e.g. related Beer–Lambert law

Metallic Materials

Refractive index of metals can be described by Drude model. It deals with electron density cloud that is fluid and a static positively charged lattice representing the metal crystal lattice.

$$n^2 = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$



$$\omega_p^2 = \frac{Ne^2}{m_e \varepsilon_0}$$ Plasma frequency

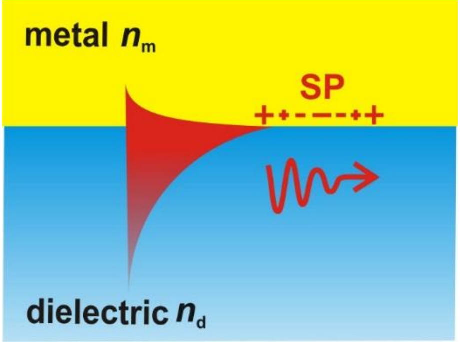
For $\omega<\omega_p$ – n is complex and radiation is attenuated.
For $\omega>\omega_p$ – n is real and radiation is not attenuated(transparent).

ω_p for Au, Ag is of 9.6, 8.5 eV and for visible wavelengths behaves as metallic (highly reflective non-transparent).

Metallic Waveguides – Surface Plasmons (SP)

Surface plasmons (SPs) or also called surface plasmon polaritons (SPPs) are waves originating from coupled oscillations of electron plasma density and associated electromagnetic field on a metal – dielectric interface.

They travel along single interface which serves a waveguide.



Propagation constant β can be analytically expressed as:

$$\beta = \frac{2\pi}{\lambda}\sqrt{\frac{n_m^2 n_d^2}{n_m^2 + n_d^2}}$$

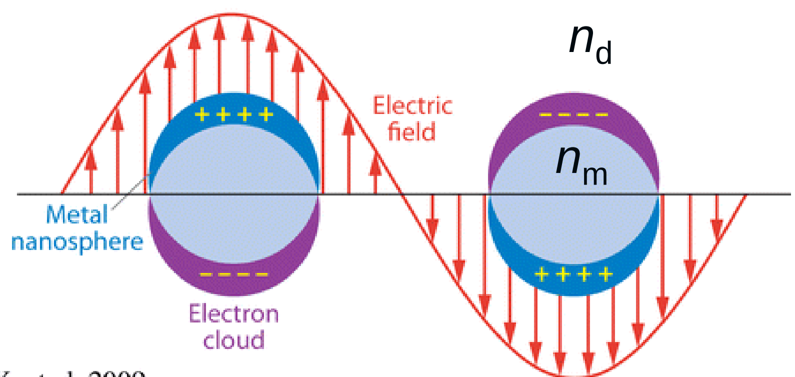
- SPs allows for tight confinement of electromagnetic field at the interface.
- For visible near infrared wavelength typically gold and silver is used where the Re{n_m^2}<0.
- Majority of the field is probing the dielectric n_d.

Localized Surface Plasmons (LSPs)

Localized surface plasmons (LSPs) are associated with electron plasma density oscillations on metallic nanoparticles. Provides unique optical / plasmonic characteristics.

Resonant effect, e.g. for spherical metallic nanoparticle with *d*<<*λ* the resonance wavelength λ_{LSPR} obeys:

$$\mathrm{Re}\{n_m^2(\lambda)\} + 2n_d(\lambda) = 0$$

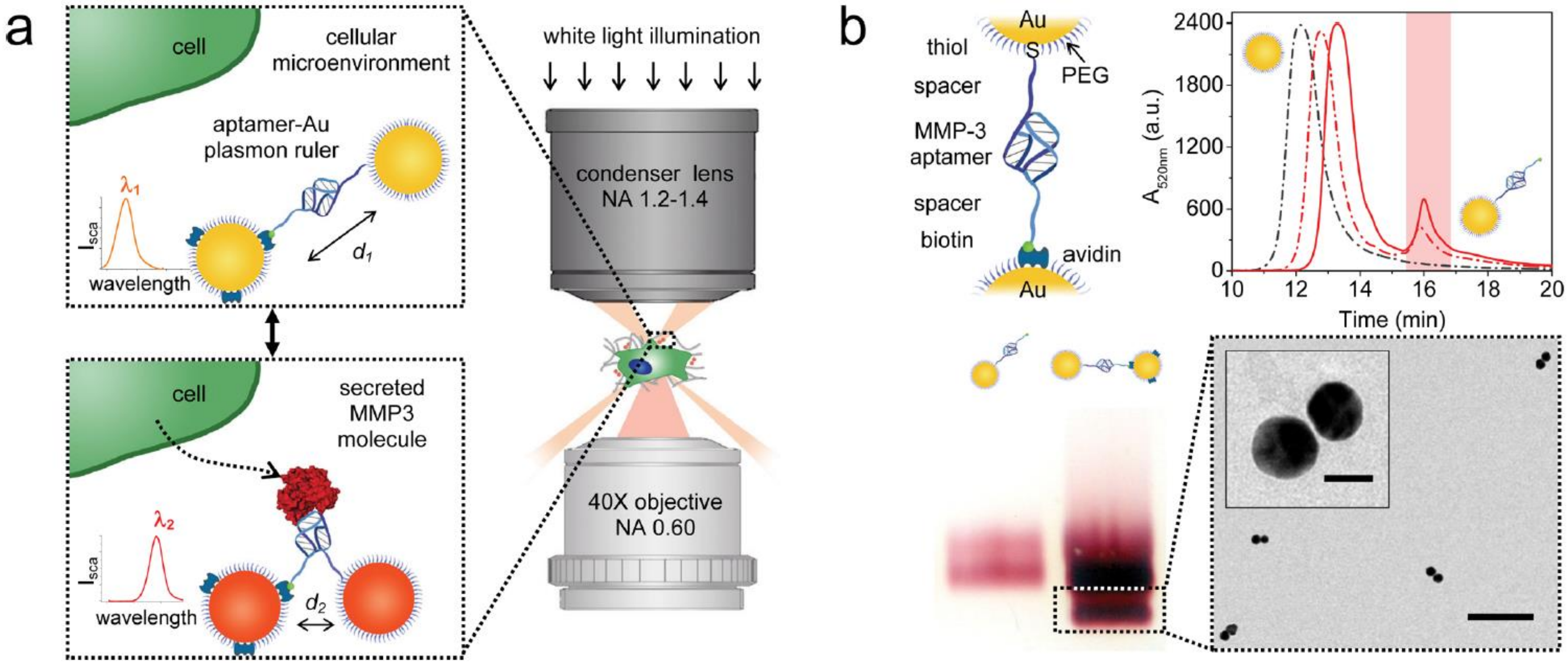


Lu X, et al. 2009.
Annu. Rev. Phys. Chem. 60:167–92

Localized surface plasmon resonance is associated with strong:

- **Absorption**
- **Scattering**
- **Field confinement and enhancement**

Example of Plasmonics in Biosensing



Concept pursued for real-time detection of growth factors, proteases…
Investigation of cellular microenvironment, concentration gradients.

Alivisatos lab: http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.5b01161

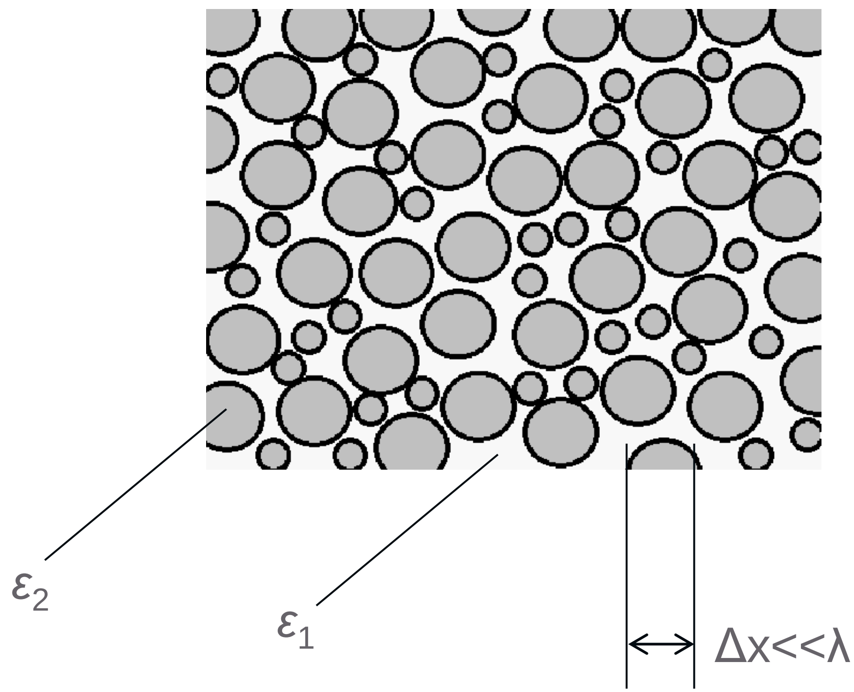
Effective Medium Theory

Refractive index of composite systems, when a material with permittivity ε_1 forms inclusions in another one with ε_2 (e.g. hydrogel layer formed by polymer networks swollen in water, biomolecules forming layers at interfaces…)

Maxwell Garnet effective medium theory:

$$\varepsilon_{eff} = \varepsilon_2 \frac{2\delta(\varepsilon_1 - \varepsilon_2) + \varepsilon_1 + 2\varepsilon_2}{\varepsilon_1 + 2\varepsilon_2 - \delta(\varepsilon_1 - \varepsilon_2)}$$

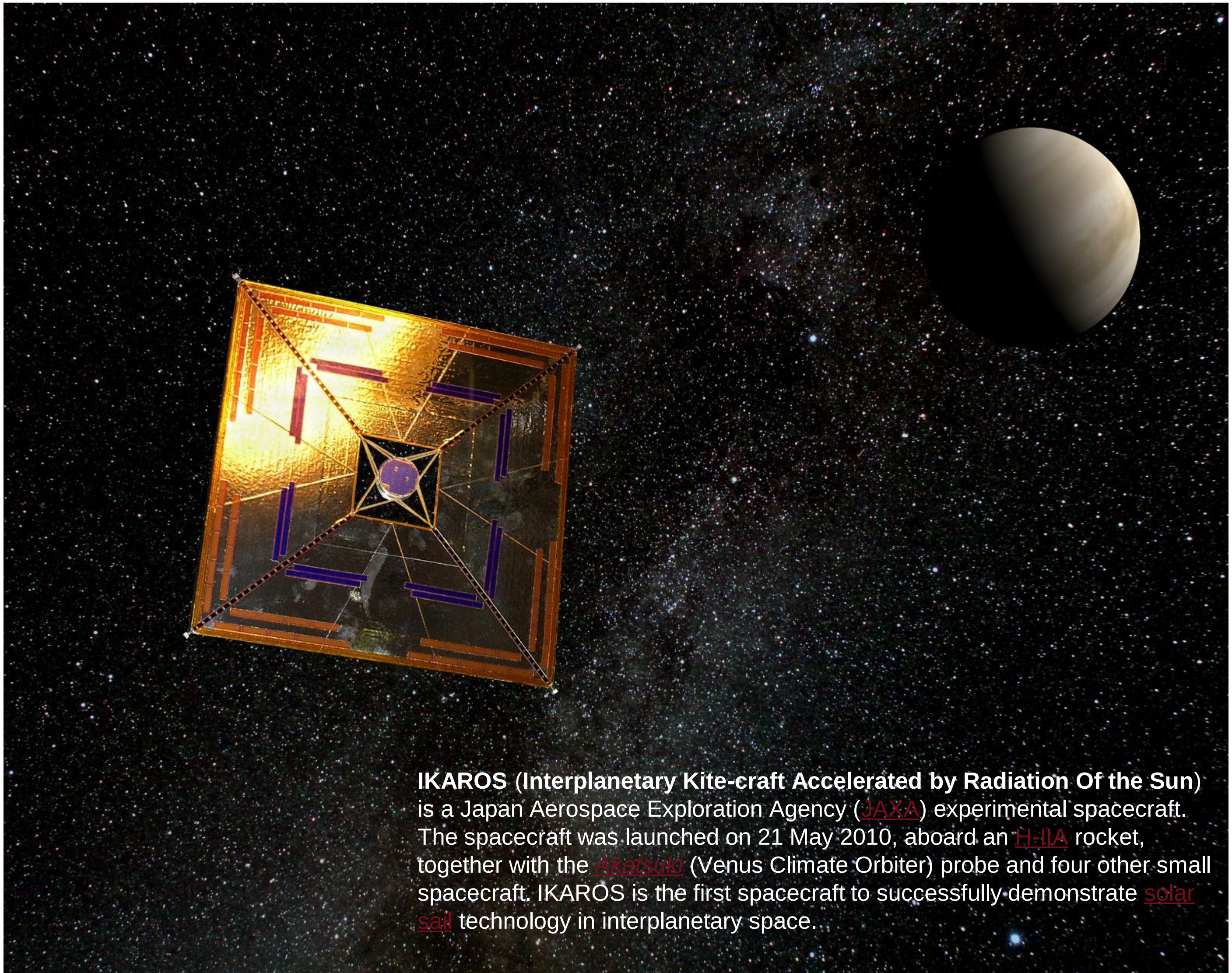
δ – volume fraction of material 1 with percolations of material 2



“Optical Tweezers”

The Nobel Prize in Physics 2018 was awarded to Arthur Ashkin, Gérard Mourou and Donna Strickland. Their inventions have revolutionised laser physics. Extremely small objects and incredibly rapid processes are now being seen in a new light. Advanced precision instruments are opening up unexplored areas of research and a multitude of industrial and medical applications.

Solar Sail



IKAROS (**Interplanetary Kite-craft Accelerated by Radiation Of the Sun**) is a Japan Aerospace Exploration Agency (JAXA) experimental spacecraft. The spacecraft was launched on 21 May 2010, aboard an H-IIA rocket, together with the Akatsuki (Venus Climate Orbiter) probe and four other small spacecraft. IKAROS is the first spacecraft to successfully demonstrate solar sail technology in interplanetary space.

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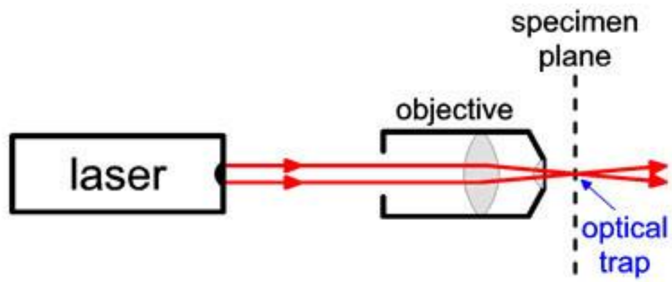
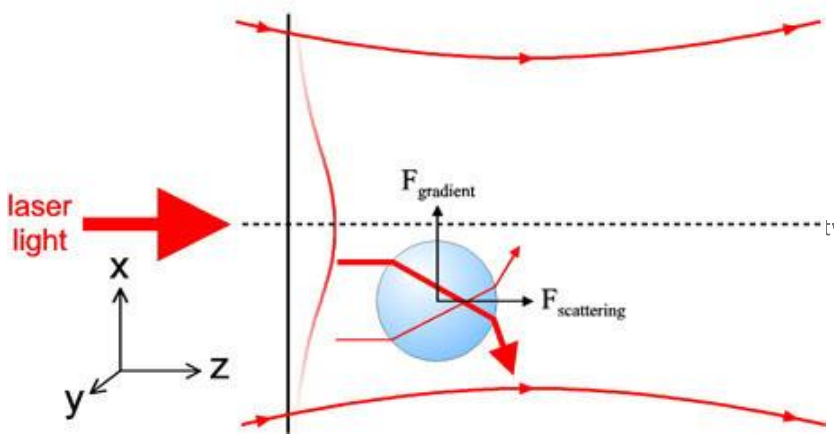
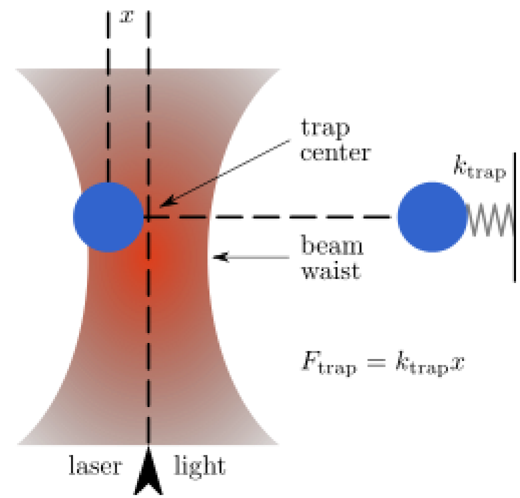
Confinement of Light Creates Optical Trap





tweezers,

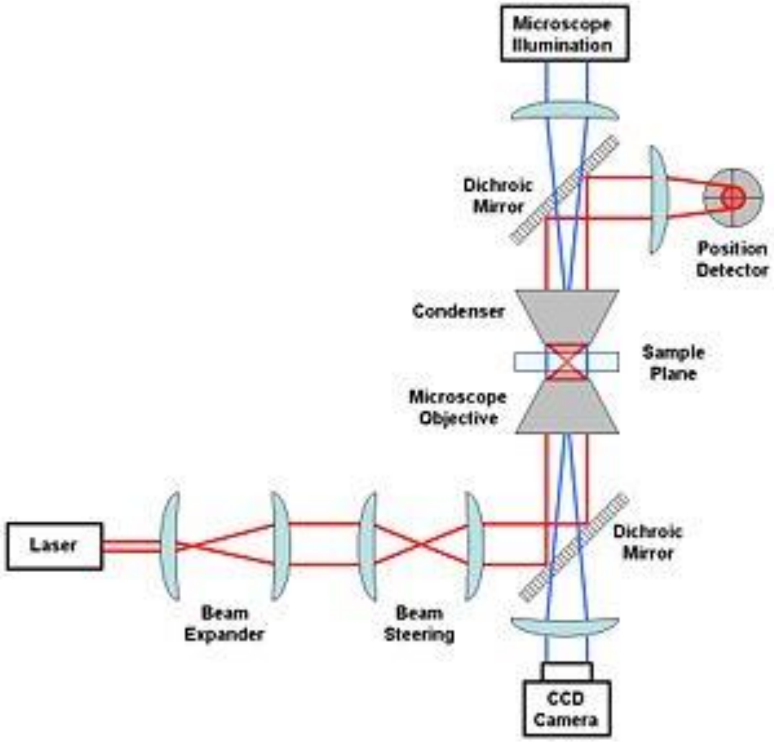
https://blocklab.stanford.edu/optical_tweezers.html

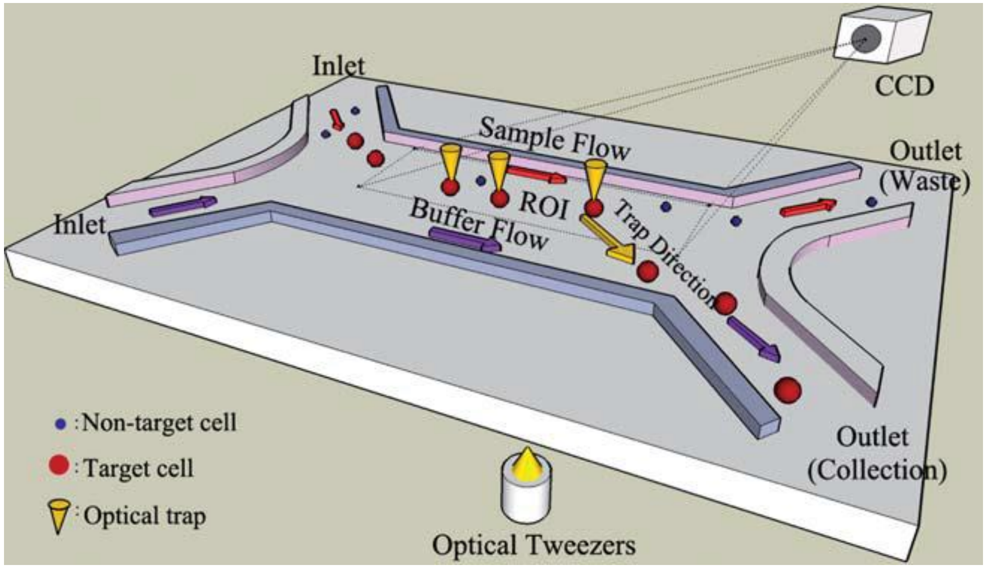


https://en.wikipedia.org/wiki/Optical_tweezers

Ashkin, A. (1970). "Acceleration and Trapping of Particles by Radiation Pressure". *Phys. Rev. Lett*. **24** (4): 156–159.

Cell Sorting

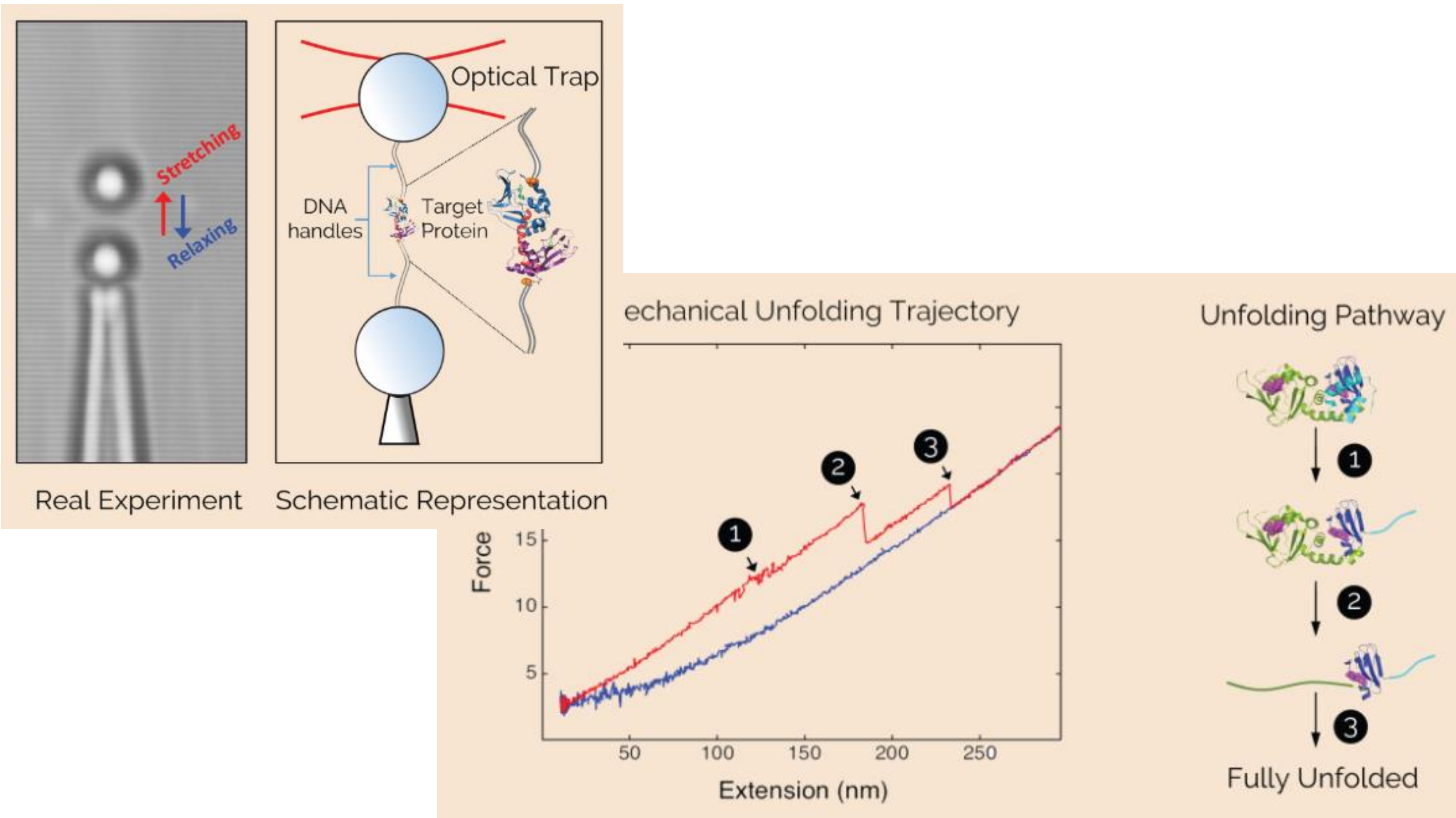




https://en.wikipedia.org/wiki/Optical_tweezers

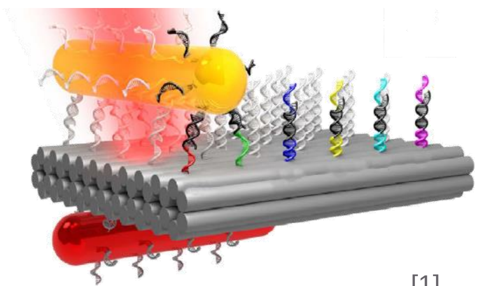
Lab Chip, 2011, 11, 3656–3662

Force Measurements



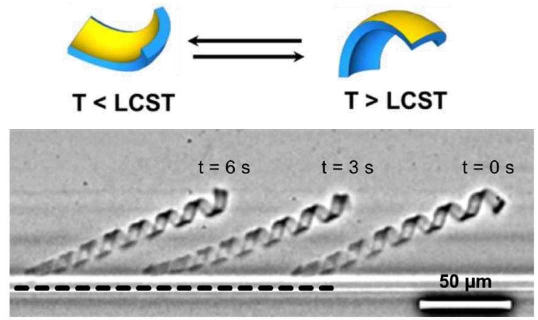
http://maillardlab.org/optical-tweezers/

Micromachines



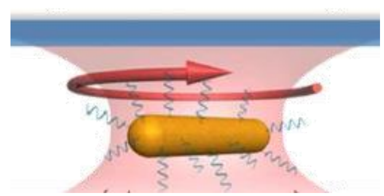
[1]

Affinity displacement reactions



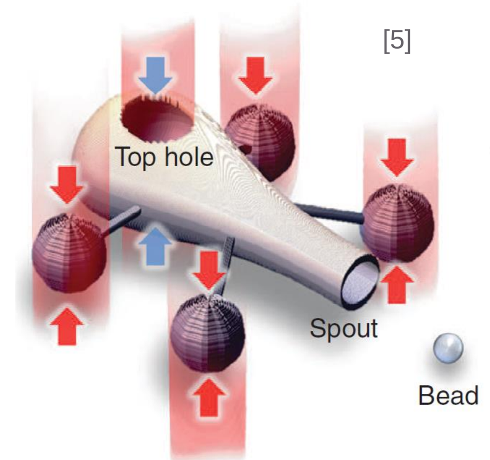
[3]

Non-reciprocal morphing



[4]

Optical torque



[5]

Optical tweezers and optical heating

[1] C. Zhou et al., Nature Commun. (2015), **6**, 8102. [3] A. Mourran et al., Adv. Mater. (2017) 29, 1604825 [4] Sipova et al, ACS Photonics, (2018), *5* (6), pp 2168–2175 [5] M. Jayson et al, Light: Sci & App (2016) 5, e16148