3.012 Fund of Mat Sci: Bonding – Lecture 1

CLASSICAL OR QUANTUM ?

Reading Material (Bonding)

Textbook: Engel and Reid, *Physical Chemistry,* Pearson (2006)

Further readings for the first half of the course (bonding); from less to more advanced (Hayden reserve, or instructor):

- **Robert Mortimer *Physical Chemistry (2nd ed),* Academic Press (2000)**
- **Atkins and de Paula *Physical Chemistry (7th ed),* Freeman & Co (2002)**
- **Thaller *Visual Quantum Mechanics* Telos (2000)**
- **Bransden & Joachain *Quantum Mechanics (2nd ed),* Prentice Hall (2000)**
- **Bransden & Joachain *Physics of Atoms and Molecules (2nd ed),* Prentice Hall (2003)**

Goal

To provide a direct, rational connection between microscopic understanding and macroscopic properties, reinforced 'just-in-time' with real-life examples in lectures and labs.

Understand what holds materials together, why they organize themselves in simple or very complex structures, and how we characterize (measure !) and describe these structures.

Such understanding is central to engineering

Advanced Materials

Photos of various research removed for copyright reasons.

Bottom-up Approach: Bonding, then Structure (4 sections, 2 weeks each)

1. Atoms (quantum)

    (3.014: Light emission in CdSe nanocrystals…)

2. Molecules (bonding)

    (3.014: XPS core electron shifts…)

3. Solids (structure: symmetry)

    (3.014: Phase transitions in piezoelectric actuators…)

4. Liquids, glasses, polymers (disorder)

    (3.014: Glass transition in acrylate polymers…)

The Master Plan for Bonding (first 2 sections):

- Discrete energy states
- The nature of the periodic table
- The scanning tunneling microscope
- The chemistry of small molecules
- The structure of carbon compounds
- Hybridization and bonding
- Exclusion principle and compressibility
- The quantization of vibrations

Homework for Fri 9

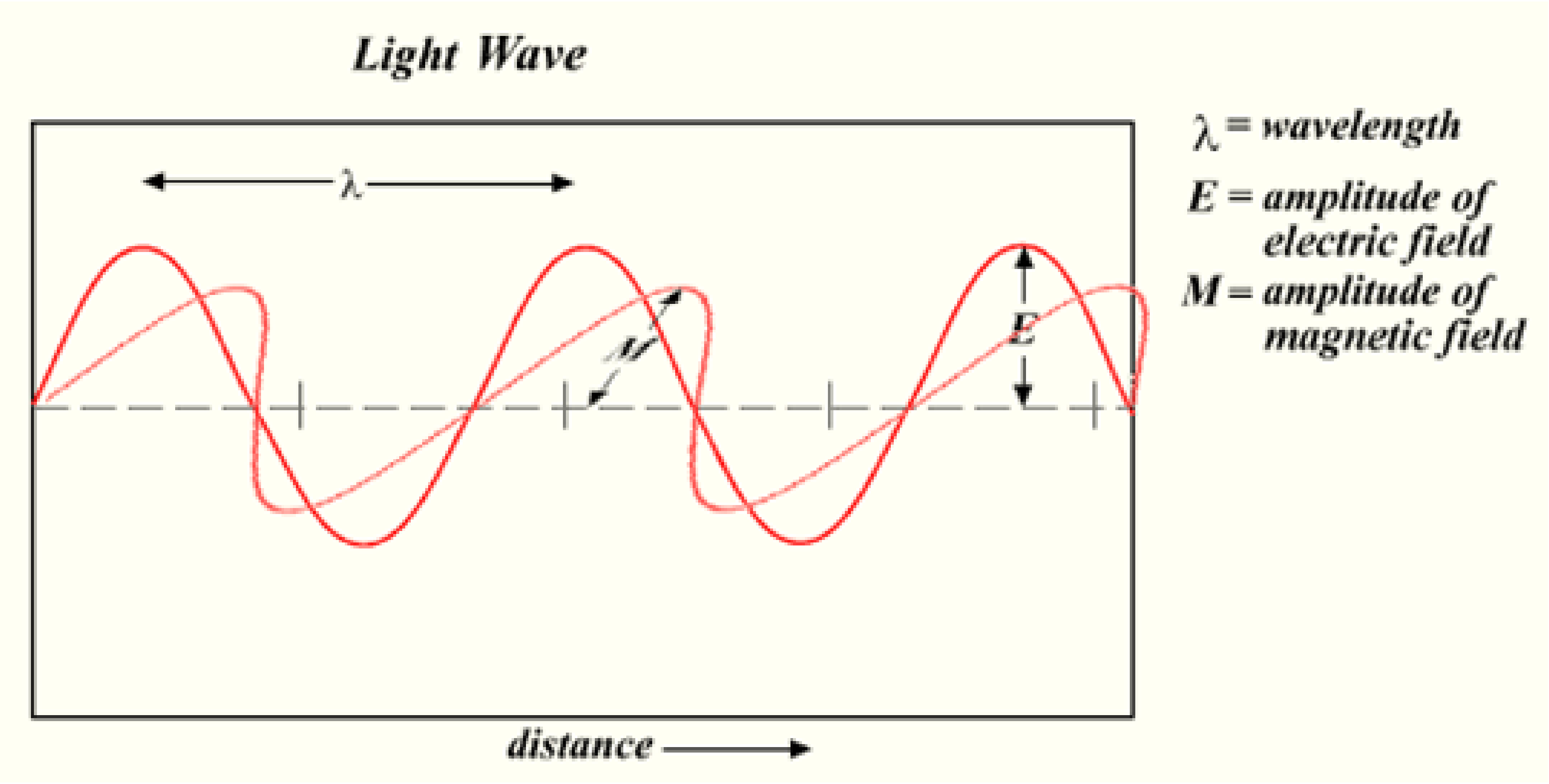
- Read: 12.1, 12.2, 12.4
- Study: 12.5, 13.2, 13.3,
- Refresh: A.1 (complex numbers)
- Problem P12.10

Round Up the Usual Suspects

- Particles and electromagnetic fields
- Forces
- Dynamics

Particles and EM Fields

Particles and EM Fields



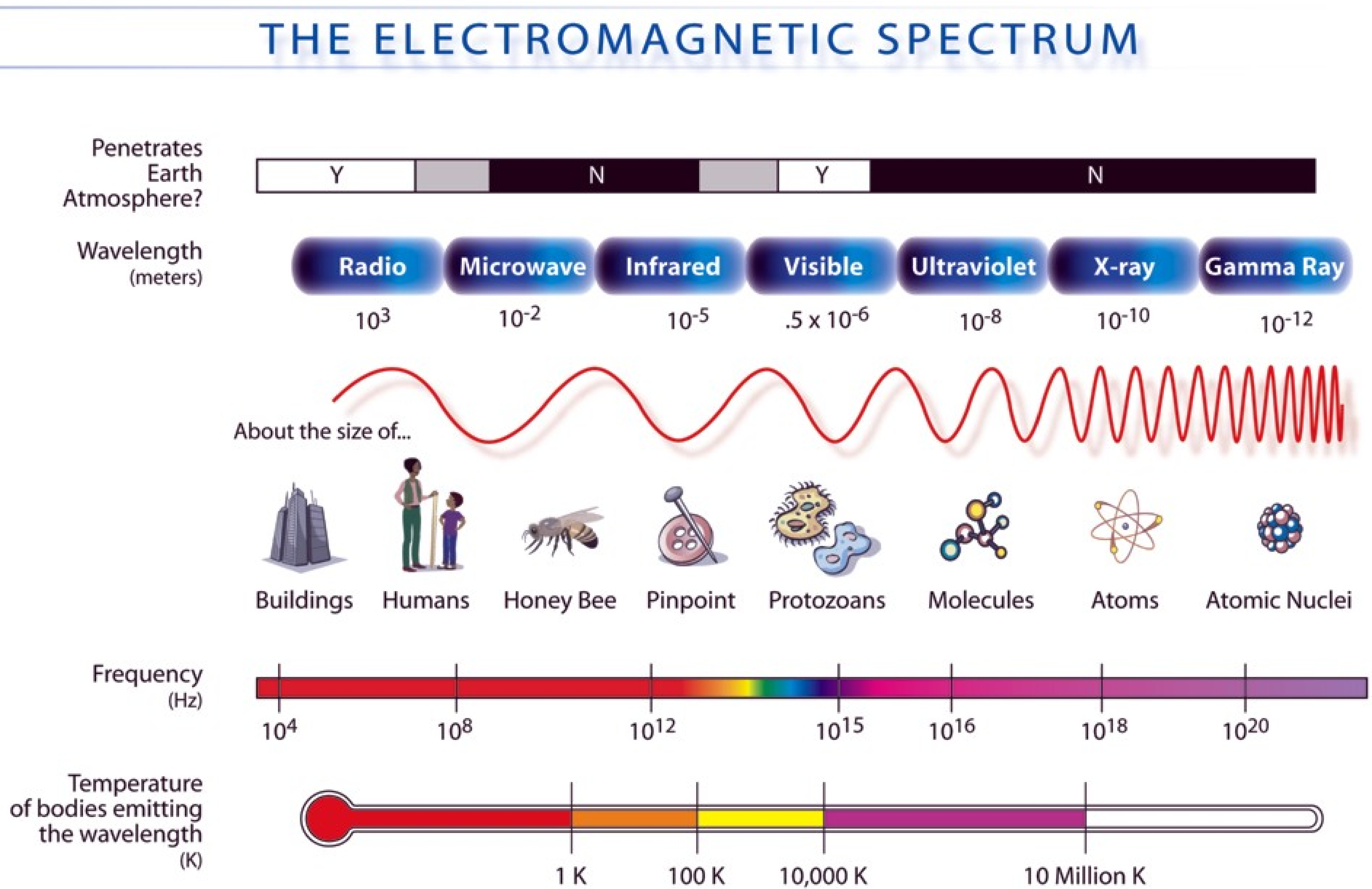
Source: Wikipedia.

Electromagnetic Waves / Photons

$$E = h\nu = h\frac{c}{\lambda} = k\mathrm{T}$$

h is Planck's constant = 6.626 10^{-34} J s

k is Boltzmann's constant = 1.381 10^{-23} J/K



Examples: http://imagers.gsfc.nasa.gov/ems/ems.html

Forces

Dynamics

Standard Model of Matter

- Atoms are made by massive, point-like nuclei (protons+neutrons)
- Surrounded by tightly bound, rigid shells of core electrons
- Bound together by a glue of valence electrons (gas vs. atomic orbitals)

Diagram of atomic structure removed for copyright reasons.

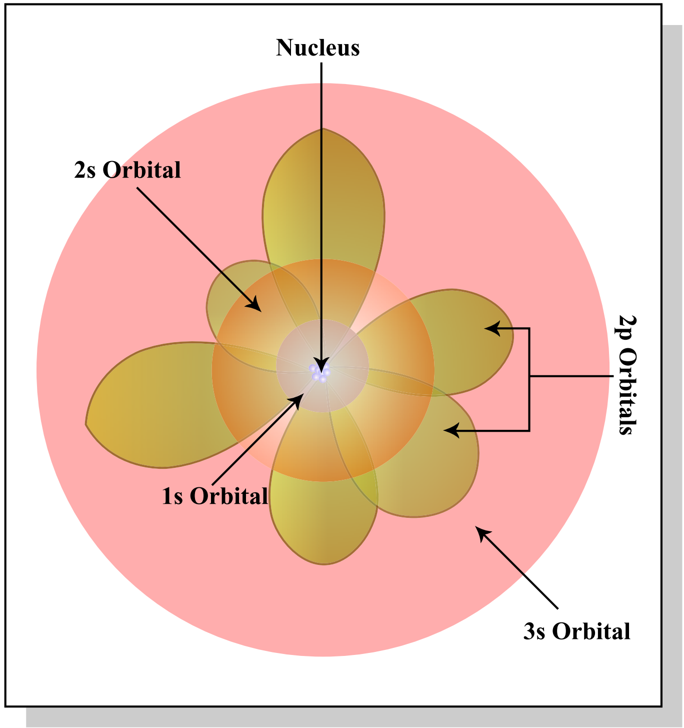


Figure by MIT OCW.

STM image of a Pt(111) Surface, by IBM.
Removed for copyright reasons.

Material Properties From First-Principles

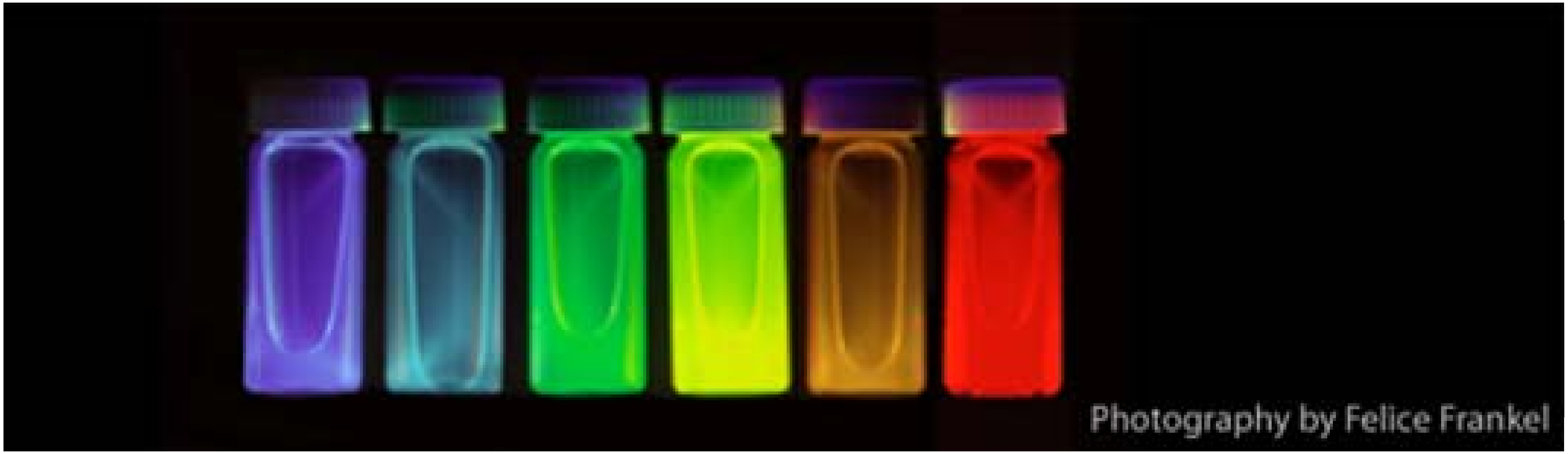
- Energy at our living conditions (300 K): 0.04 eV (kinetic energy of an atom in an ideal gas).
- Differences in bonding energies are within one order of magnitude of 0.29 eV (hydrogen bond).
- Binding energy of an electron to a proton (hydrogen): 13.6058 eV = 0.5 atomic units (a.u)
- Everything, from the muscles in our hands to the minerals in our bones is made of atomic nuclei and core electrons bonded together by valence electrons (**standard model** of matter)

Why do we need quantum mechanics ?

Structural properties (fracture in silicon)

Image of a propagating fracture in silicon, removed for copyright reasons.

Electronic, optical, magnetic properties

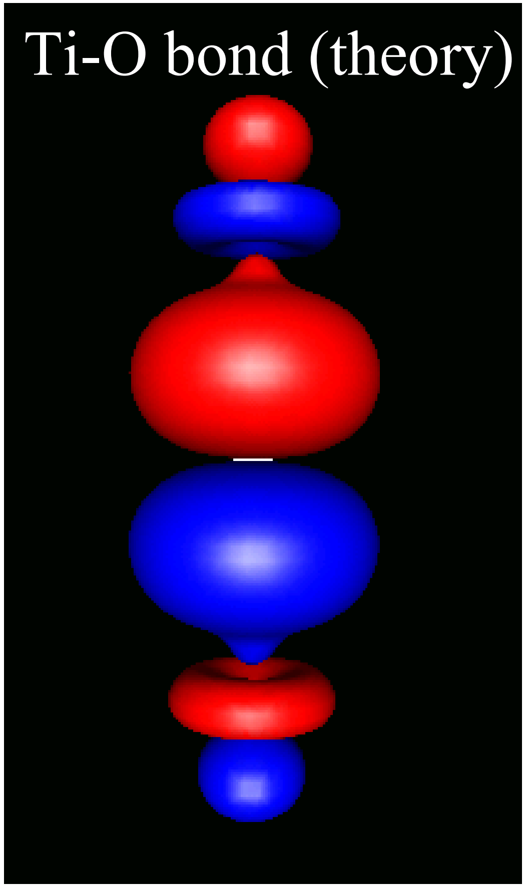


It's for real…

Cu-O bond (experiment !)

Experimental image of a Copper-Oxygen Bond in Cuprite, removed for copyright reasons.

See Zuo, J. M., M. Kim, M. O'Keeffe, and J. C. H. Spence. "Direct observation of d-orbital holes and Cu–Cu bonding in Cu_2O." *Nature* 401 (1999): 49 - 52.



… and it makes it to the NYTimes

Scanned image of a New York Times article removed for copyright reasons.

See Browne, Malcom W. "Glue of Molecular Existence Is Finally Unveiled." *New York Times*, September 7, 1999, p. 5.

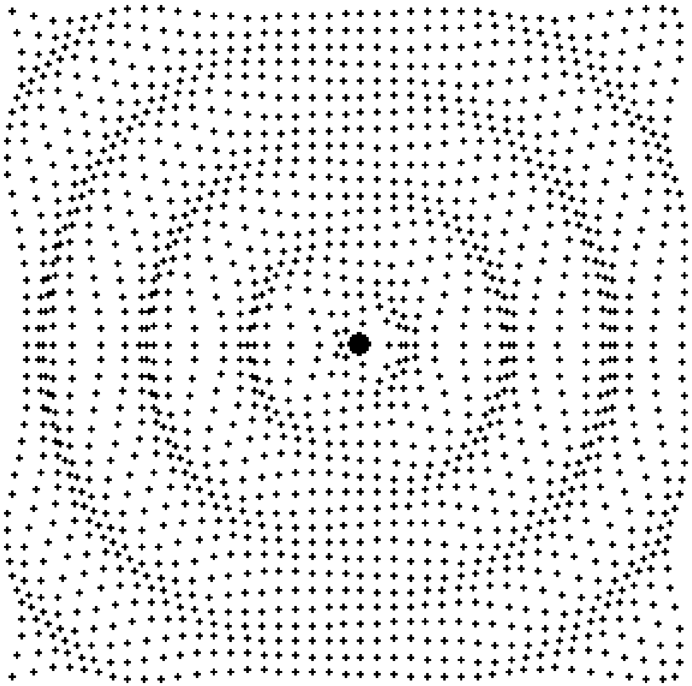
Mechanics of a Particle

$$m\frac{d^2\vec{r}}{dt^2} = F(\vec{r}) \longrightarrow \begin{array}{c} \vec{r}(t) \\ \vec{v}(t) \end{array}$$

The sum of the kinetic and potential energy (E=T+V) is conserved

Photo of two circular waves overlapping. Image removed for copyright reasons.

Description of a Wave



The wave is an excitation (a vibration): We need to know the amplitude of the excitation at every point and at every instant

$$\Psi = \Psi(\vec{r}, t)$$

Principle of Linear Superposition

Photo courtesy of Spiralz.

Interference patterns

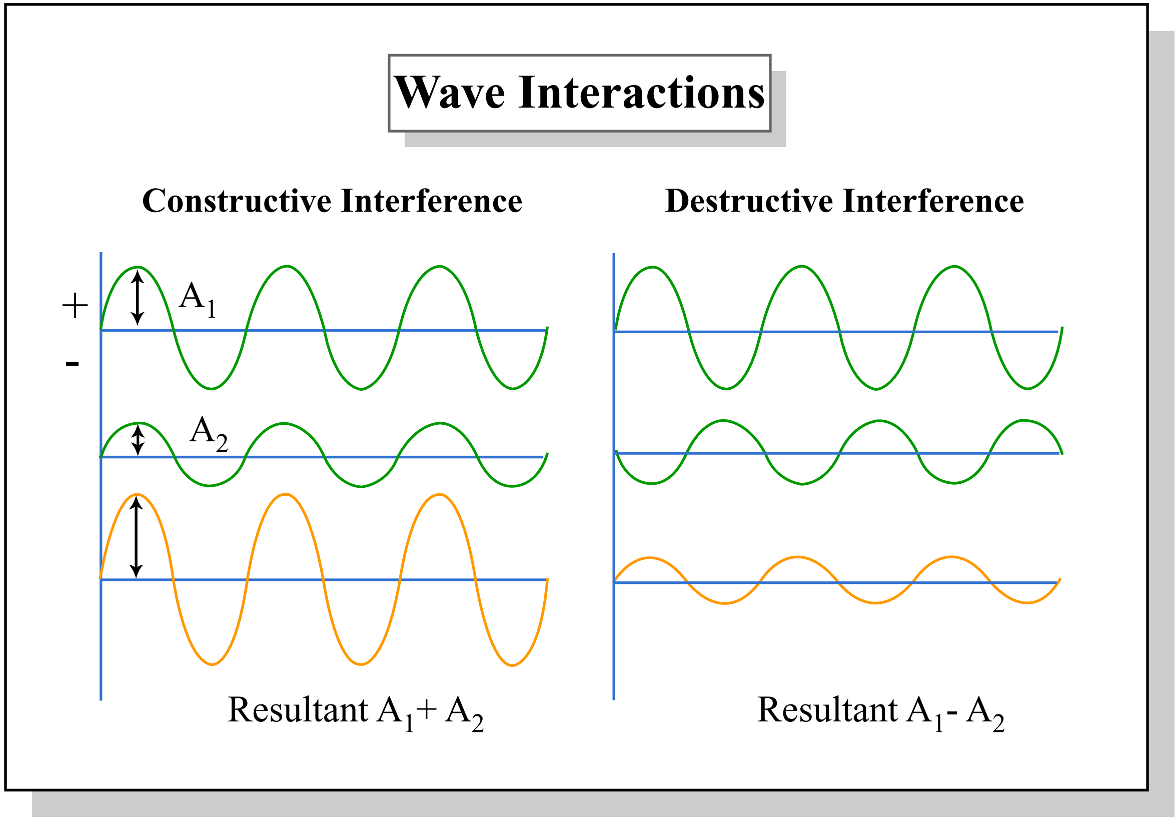


Figure by MIT OCW.

Interference in Action

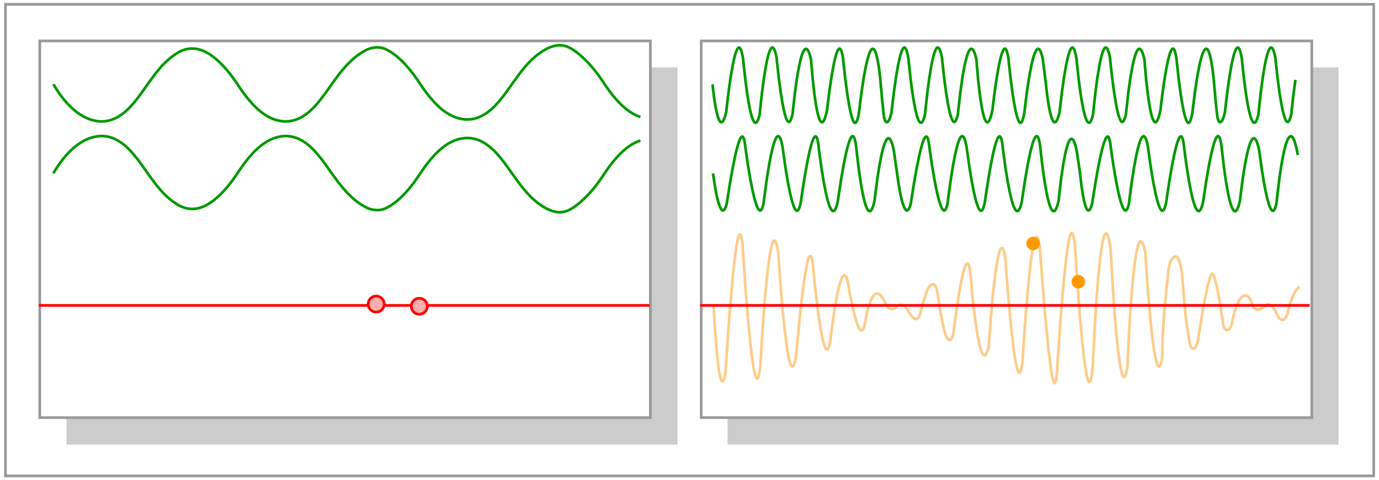


Figure by MIT OCW.

Interference in Action

Photo of Irving Langmuir and Katherine Blodgett, removed for copyright reasons.

Photo of a Contax camera, with anti-reflective coating first developed by Carl Zeiss.
Photo removed for copyright reasons.

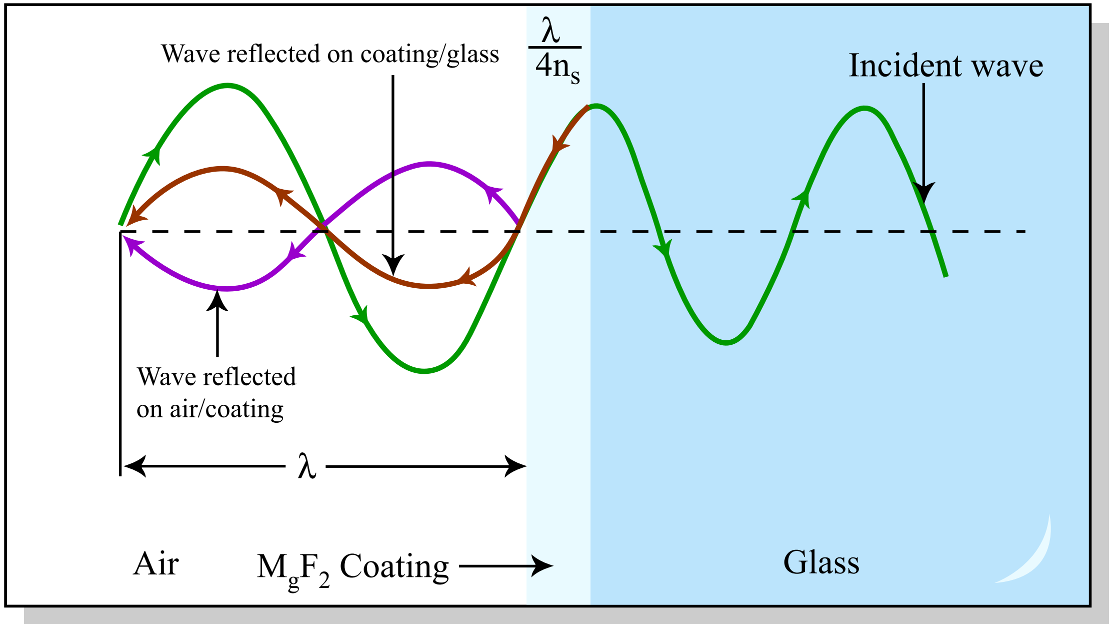


Figure by MIT OCW.

Wave-particle Duality

- *Waves have particle-like properties:*
  - *Photoelectric effect: quanta (photons) are exchanged discretely*
  - *Energy spectrum of an incandescent body looks like a gas of very hot particles*

Diagrams of the photoelectric effect and of a P-N solar cell, removed for copyright reasons.

Wave-particle Duality

- Particles have wave-like properties:
  - Quantum mechanics: Electrons in atoms are standing waves – just like the harmonics of an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926…)

When is a particle like a wave ?

Wavelength • momentum = Planck

$$\updownarrow$$

Image of the double-slit experiment removed for copyright reasons.

See the simulation at http://www.kfunigraz.ac.at/imawww/vqm/movies.html:

"Samples from *Visual Quantum Mechanics*": "Double-slit Experiment."

$$\lambda \bullet p = h$$

$$(h = 6.626 \times 10^{-34} \text{ J s} = 2\pi \text{ a.u.})$$