\[ E_{\text{kin}} = \hbar \omega - \phi - E_b \]
\( \vec{A} \): vector potential of incident light

\( \psi \): incident angle

\( \vartheta \): polar angle of emission

\( \varphi \): azimuthal angle of emission

\( E_{\text{kin}} \): kinetic energy of emitted electron

\( \vec{p} = \hbar \vec{k} = \hbar \frac{2\pi}{\lambda} \vec{e}_k \): momentum of emitted electron

\( \vec{\sigma} \): spin of emitted electron
K. M. Siegbahn

Nobel price in physics 1981 for Siegbahn (shared with Bloembergen and Schawlow) “for his contribution to the development of high-resolution electron spectroscopy".

The Orbitron gallery of atomic orbitals
Binding Energy vs Atomic # vs Electron Configuration
hemispherical energy analyzer
Three-step model

1. Photoexcitation
2. Transport
3. Escape

VL, FL: Valence Band

Secondary Emission
Oxidized InAs

XPS Intensity

Binding Energy (eV)

As 2p
In 3p
O 1s
In 3d
C 1s
As 3p
As 3d

As LMM

In 3d

3d_{5/2}
3d_{3/2}
Chemical shift in XPS

Example:
C 1s XPS signal in ethylfluoroacetate

\[
\begin{align*}
\text{F} & \quad \text{C} & \quad \text{C} & \quad \text{O} & \quad \text{H} & \quad \text{H} & \quad \text{H} \\
\text{F} & \quad \text{C} & \quad \text{C} & \quad \text{O} & \quad \text{C} & \quad \text{H} & \quad \text{H} \\
\end{align*}
\]

\[E_B = 291.2 \text{ eV}\]

[Graph showing XPS spectra for different Cu compounds]

- NaCuO\(_2\): Cu\(^{3+}\)
- CuO: Cu\(^{2+}\)
- Cu\(_2\)O: Cu\(^{1+}\)
- Cu metal: Cu\(^{0+}\)
UPS

Cu(110) / θ = 0° (Normal emission)
\( \hbar \omega = 21.2 \text{ eV} \)

Diagram showing energy distribution and binding energy with notations for peak labeling.
ARPES principle

$$K = \frac{p}{\hbar} = \sqrt{2mE_{\text{kin}} / \hbar}$$

- $$K_x = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}}} \sin \vartheta \cos \varphi$$
- $$K_y = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}}} \sin \vartheta \sin \varphi$$
- $$K_z = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}}} \cos \vartheta$$

Vacuum

$$E_{\text{kin}} = h\nu - |E_B| - \Phi$$

$$\vec{K} = \vec{k}_{\parallel} + \vec{k}_{\text{photon}}$$

Solid

$$E_B$$

conservation of parallel momentum
ARPES on graphene
Inverse photoemission spectroscopy

Fig. 12.19. Electronic levels and recombination processes for inverse photoemission (a) and photoemission and inverse photoemission for C\textsubscript{60} (1) and K\textsubscript{3}C\textsubscript{60} (2) (b); The Mullikan symbols $h_{u}$ and $t_{1u}$ label the symmetry of the bands; (b) after [12.15].
Two-photon photoemission (2PPE)
X-ray adsorption spectroscopy

Figure 2.3: The absorption cross-section $\mu/\rho$ for several elements over the x-ray energy range of 1 to 100 keV. Notice that there are at least 5 orders of magnitude in variation in $\mu/\rho$, and that in addition to the strong energy dependence, there are also sharp rises corresponding to the core-level binding energies of the atoms.
Figure 2.5: Decay of the excited state: x-ray fluorescence (left) and the Auger effect (right). In both cases, the probability of emission (x-ray or electron) is directly proportional to the absorption probability.
XAS experimentally

- **Transmission mode:** \( I(\hbar \nu) = I_0 e^{-\mu z} \)

- **Fluorescence Yield** (bulk sensitive, but often saturation problems)

- **Total Yield (TY):**
  - All (in-) elastic photoelectrons
  - Probing depth: 40Å to 100Å
  - Good signal to noise ratio (I~100 pA)

- **Partial Electron Yield (PEY):**
  - Only photo electrons with \( E_{\text{kin}} \geq E_{\text{threshold}} \), i.e. elastic photo electrons (ca. 5% of TY-signal)
  - Probing depth: ~15Å (surface)

All methods can be measured simultaneously to get more information
Figure 2.6: XAFS $\mu(E)$ for FeO. On top, the measured XAFS spectrum is shown with the XANES and EXAFS regions identified. On the bottom, $\mu(E)$
The Universal Curve for the Electron Mean Free Path

![Graph showing the universal curve for the electron mean free path. The y-axis represents the inelastic mean free path in Å, and the x-axis represents electron energy in eV. The graph includes a curve and numerous data points.](image)
Dipole radiation

Dipole antenna (harmonic oscillation of charge) with induced E- and B-field

Emission characteristics (A=intensity)

3D-view
Electrons on circular orbit

nonrelativistic

radius
acceleration
electron
radiation field
electron trajectory

relativistic

opening angle $\theta$

Radiation Power $P$

$$P = \frac{2}{3} \frac{e^2 c}{R^2} \beta^4 \left( \frac{E}{m_0 c^2} \right)^4 \gamma$$

nonrelativistic:

$\rightarrow v << c \rightarrow \beta << 1$

$\Rightarrow$ Radiation power is very small and emitted in all directions

E = particle energy
$R = \text{radius of curvature}$
$m_0 = \text{particle mass}$

$$\beta = \frac{v}{c}; \gamma = \frac{E}{m_0 c^2}$$

Relativistic:

$\rightarrow v \approx c \rightarrow \beta \approx 1$

$$P = \frac{2}{3} \frac{e^2 c}{R^2} \gamma^4$$

$\Rightarrow$ extremely high radiation power, emitted in a sharp forward cone!
Generation of Synchrotron Radiation

1. emission of electrons by an electron gun
2. acceleration in a linear accelerator (LINAC)
3. transmission to a circular accelerator (booster synchrotron) to reach the required energy level (e.g. E = 6 GeV at ESRF) → relativistic electrons
4. injection of high energy electrons into a large storage ring (circumference e.g. 844 m at ESRF) where they circulate in vacuum at a constant energy for many hours

Velocity of relativistic electrons (6 GeV) $v$ is only 107 cm/s slower than the velocity of light
Storage rings and beamlines
Angular distribution (relativistic)

Example:
E = 6 GeV, \( v \) is only 107 cm/s slower than the velocity of light (\( c \approx 3 \times 10^{10} \) cm/s)
\( \gamma = \frac{E}{mc^2} \approx 1820 \)
\( \theta \approx 8 \times 10^{-5} \) rad (0.08 mrad)
The emitted radiation is a sharp cone with an opening angle \( \theta \approx 0.08 \) mrad

\( \Rightarrow \) Excellent collimation!
\( \Rightarrow \) in a distance of 50 m from the source, one obtains a spot of only \( \sim 4 \) mm!
Pulse duration and energy spectrum

Duration of radiation flash (single electron):

\[ \Delta t = \frac{4R}{3c\gamma^3} \]

\[ E_c(keV) = 0.665B(T)E(GeV)^2 \]

\[ \lambda_c = 5.59 \cdot \frac{R}{E^3} \]
Charaterize the properties of a Synchrotron Radiation source

Total flux \equiv \frac{\text{Photons}}{\text{s}}

Spectral flux = \frac{\text{Total flux}}{0.1\%\text{bandwidth}} \left[ \frac{\text{Photons/s}}{0.1\%\text{bandwidth}} \right]

Brightness = \frac{\text{Total flux}}{\text{solid angle} \cdot 0.1\%\text{bandwidth}} \left[ \frac{\text{Photons/s}}{\text{mrad}^2 \cdot 0.1\%\text{bandwidth}} \right]

Brilliance = \frac{\text{Total flux}}{\text{solid angle} \cdot \text{source area} \cdot 0.1\%\text{bandwidth}} \left[ \frac{\text{Photons/s}}{\text{mrad}^2 \cdot \text{mm}^2 \cdot 0.1\%\text{bandwidth}} \right]

Brilliance is the figure of merit for the design of new Synchrotron Radiation sources.
Extremely high intensity, broad energy range

Emission spectrum

Number of photons vs. Wavelength (Å)

- Sun
- X-ray tubes
- Bending magnet

Energy vs. Number of photons

- 1 eV
- 10 eV
- 100 eV
- 1 keV
- 10 keV
- 100 keV

Brilliance (photons/s/mm²/mrad²/0.1%BW)

- 1900
- 1920
- 1940
- 1960
- 1980
- 2000

ESRF (future)
ESRF (2000)
ESRF (1994)

1st generation
2nd generation
3rd generation

Free electron lasers

Synchrotron radiation

Emission spectrum

Wavelength (Å) vs. Number of photons

10⁷ 10⁸ 10⁹ 10¹⁰ 10¹¹ 10¹² 10¹³

1 eV 10 eV 100 eV 1 keV 10 keV 100 keV

Energy vs. Number of photons

10⁷ 10⁸ 10⁹ 10¹⁰ 10¹¹ 10¹² 10¹³ 10¹⁴ 10¹⁵ 10¹⁶ 10¹⁷ 10¹⁸ 10¹⁹ 10²⁰ 10²¹ 10²² 10²³
Magnetic wigglers and undulator (N periods)

Principle:
periodic arrangement of short bending magnets of alternating polarity perpendicular to the plane of the storage ring

Permanent magnetic materials e.g. Nd-Fe-B

⇒ force the electrons to oscillate („wiggle“) perpendicular to their direction of motion
⇒ Radiation is emitted during each individual wiggle
⇒ increase of the intensity
wiggler and undulator

Wiggler regime: $\alpha > 1/\gamma$

Undulator regime: $\alpha \sim 1/\gamma$

In the undulator regime the radiation cones overlap and the wave trains can interfere
Forms of Synchrotron Radiation

- Bending magnet radiation
- Wiggler radiation
- Undulator radiation
Examples of Wigglers and Undulators
Evolution of Brilliance

1st generation: Exploitation of the light from the bending magnets of e+/e- colliders originally built for elementary particle physics

2nd generation: Radiation from bending magnets and introduction of first insertion devices, lower e-beam emittance, optimization of light extraction

3rd generation: Dedicated storage rings, very low e-beam emittance, brilliance is figure of merit, mainly undulators, long straight sections
Evolution of Source Brilliance

Brilliance =
Spectral flux
source area x solid angle

Spring8

APS

ESRF

PETRA III
under construction

Source size

3rd generation SRS

2nd generation SRS

1st generation SRS

X-ray tubes

Year

1920 1940 1960 1980 2000

Brilliance

$10^6$ $10^9$ $10^{12}$ $10^{15}$ $10^{18}$

Divergence
European Synchrotron Radiation Facility (ESRF)
Beamline organization

LINAC (Linear Accelerator)

Storage ring
(2.5 Gev / 450 mA)

Bending Magnet

Si(111) Double Crystal Monochromator

Cylindrical mirror
to sample position
How does a beamline work?
Basic principle of monochromator:
Bragg reflection from perfect single crystal

\[ 2d_{hkl} \sin \theta = n\lambda \]
Energy range of standard monochromator

Bragg Reflection
- Si 111
- Si 311
- Si 511

Bragg angles 3°~27°

Energy range 4.4~110 keV

Photon energy (wavelength) can be selected by crystal, net planes, and Bragg angle.

[Graph showing Bragg angles and photon energy vs. Bragg angle]
Double crystal monochromator

Problems with single crystal monochromators
- the monochromatic beam moves when the energy is changed
- high harmonic content
- big tails

Solution: double crystal design!
Simplest design: cutting a channel for the beam in a silicon block (channel cut monochromator)

- Use the same crystals and $d$-spacing for 1$^{st}$ and 2$^{nd}$ crystals
- Keep parallel setting
refractive index: \( n = 1 - r_0 \rho \lambda^2 / 2\pi - i \mu \lambda / 4\pi \)

By Snell’s law \((n_1 \cos(\theta_1) = n_2 \cos(\theta_2))\) with \( \theta \) the grazing angle) in the absence of absorption (total reflection), we find total external reflection for angles less than \( \theta_c \approx \lambda (r_0 \rho / \pi)^{1/2} \)

\( \theta_c \) typically a few mrad for x-ray mirrors

Surface roughness must be considered around critical energy (angle).
Bent mirrors (focusing and collimating)

Focusing of the x-ray beam \( \rightarrow \) reflecting surface must have some curvature (achieved e.g. by bending mirror, \textbf{mirror focuses in one plane only!})

Bending radius \( R \) (can be \( \sim 10 \) km)

\[
R = \frac{2D_1D_2}{\theta(D_1 + D_2)}
\]

imaging the source in the vertical direction with unity magnification (1:1 focusing)

1:1 focusing

improving energy resolution of a following monochromator by production of a parallel beam (collimating)
Free electron laser (FEL)

Figure 1. Comparison of several recently commissioned FELs (FLASH and LCLS) and several planned FELs (sFLASH, Euro XFEL, NLS) with a state-of-the-art undulator beamline on the Diamond Light source. The standard definition of brightness is given in photons/unit time/unit solid angle/unit area/normalised bandwidth. Courtesy of STFC, New Light Source Conceptual Design Report (2010) [1].
SASE – spontaneous amplified self-emission

Linac-based Free Electron Laser
Self-Amplified Spontaneous Emission (SASE)

Principle design (SPring-8, Japan):

- **e-gun** (pulsed)
- **linac** (linear accelerator)
- **undulator**

The e-beam is generated by the e-gun and accelerated through the linac. It then enters the undulator, where micro-bunching occurs, leading to the amplification of the X-Ray Laser. The process is depicted in the diagram.
Snapshots for different times after excitation ("pump-probe experiment") \implications "film" of the reaction
Obstacle: Coulomb-Explosion

Example: Lysozyme

Requirement: Pulse must be short enough and not too intense, to take picture before molecule disintegrates!
This is a focused beam of synchrotron x-rays emerging through a thin window and ionizing the air to give a blue light.
Crab Nebula – an astronomical synchrotron source

The supernova exploded in 1054 AD, and the gas should have cooled by today. But it is still emitting UV and X-rays. Why? The answer is that very high energy electrons in a weak magnetic field are emitting synchrotron radiation.
RF-cavities in the ring provide the electric field to accelerate the electrons to compensate for the radiation losses

\[ v_{RF} = 352 \text{ MHz} \]

This means:
992 buckets of stable phase for the electrons

A bucket filled with electrons is called a **bunch** (duration 10-100ps).

\[ \Delta t = \frac{1}{c} \cdot \frac{1}{N} = 2.84 \text{ ns} \quad (\text{flashes}) \]
Time structure of Synchrotron Radiation

By selecting well defined time structure

→ Time resolved measurements (e.g. dynamic processes in Biology, chemical bonding, magnetism and Mössbauer spectroscopy with Synchrotron Radiation

→ Mode of operation depends on the type of experiment
Figure 2.3: The absorption cross-section $\mu/\rho$ for several elements over the x-ray energy range of 1 to 100 keV. Notice that there are at least 5 orders of magnitude in variation in $\mu/\rho$, and that in addition to the strong energy dependence, there are also sharp rises corresponding to the core-level binding energies of the atoms.
Figure 2.5: Decay of the excited state: x-ray fluorescence (left) and the Auger effect (right). In both cases, the probability of emission (x-ray or electron) is directly proportional to the absorption probability.
XAS experimentally

- **Transmission mode:**  \( I(h\nu) = I_0 e^{-\mu z} \)

- **Fluorescence Yield** (bulk sensitive, but often saturation problems)

- **Total Yield (TY):**
  All (in-) elastic photoelectrons
  ● Probing depth: 40Å to 100Å
  ● Good signal to noise ratio (I~100 pA)

- **Partial Electron Yield (PEY):**
  Only photo electrons with \( E_{\text{kin}} \geq E_{\text{threshold}} \), i.e. elastic photoelectrons (ca. 5% of TY-signal)
  ● Probing depth: ~15Å (surface)

All methods can be measured simultaneously to get more information
Figure 2.6: XAFS $\mu(E)$ for FeO. On top, the measured XAFS spectrum is shown with the XANES and EXAFS regions identified. On the bottom, $\mu(E)$
The Universal Curve for the Electron Mean Free Path
Dipole radiation

Dipole antenna (harmonic oscillation of charge) with induced E- and B-field

Emission characteristics (A=intensity)

3D-view
Electrons on circular orbit

**nonrelativistic**
- $v \ll c \rightarrow \beta \ll 1$
- Radiation power is very small and emitted in all directions

**relativistic**
- $v \approx c \rightarrow \beta \approx 1$
- Extremely high radiation power, emitted in a sharp forward cone!

**Radiation Power $P$**

\[ P = \frac{2}{3} \frac{e^2 c}{R^2} \beta^4 \left( \frac{E}{m_0 c^2} \right)^4 \gamma \]

- $E =$ particle energy
- $R =$ radius of curvature
- $m_0 =$ particle mass

**Equations:**

\[ \beta = \frac{v}{c}; \quad \gamma = \frac{E}{m_0 c^2} \]
Generation of Synchrotron Radiation

1. emission of electrons by an electron gun
2. acceleration in a linear accelerator (LINAC)
3. transmission to a circular accelerator (booster synchrotron) to reach the required energy level (e.g. E = 6 GeV at ESRF) → relativistic electrons
4. injection of high energy electrons into a large storage ring (circumference e.g. 844 m at ESRF) where they circulate in vacuum at a constant energy for many hours

Velocity of relativistic electrons (6 GeV) $v$ is only 107 cm/s slower than the velocity of light
Storage rings and beamlines
Angular distribution (relativistic)

Example:
$E = 6 \text{ GeV}$, $v$ is only $107 \text{ cm/s}$ slower than the velocity of light ($c \approx 3 \times 10^{10} \text{ cm/s}$)

$\gamma = \frac{E}{mc^2} \approx 1820$

$\theta \approx 8 \times 10^{-5} \text{ rad} \ (0.08 \text{ mrad})$

The emitted radiation is a sharp cone with an opening angle $\theta \approx 0.08 \text{ mrad}$

$\Rightarrow$ Excellent collimation!
$\Rightarrow$ in a distance of 50 m from the source, one obtains a spot of only $\sim 4 \text{ mm}$!
Pulse duration and energy spectrum

Duration of radiation flash (single electron):

$$\Delta t = \frac{4R}{3c\gamma^3}$$

Electric Field

Flux

Critical Energy

Half of power emitted below

Half of power emitted above

$$E_c(keV) = 0.665B(T)E(GeV)^2$$

$$\lambda_c = 5.59 \cdot \frac{R}{E^3}$$

broad energy spectrum!
Charaterize the properties of a Synchrotron Radiation source

Total flux ≡ \( \frac{\text{Photons}}{s} \)

Spectral flux = \( \frac{\text{Total flux}}{0.1\% \text{ bandwidth}} \) \( \left[ \frac{\text{Photons/s}}{0.1\% \text{ bandwidth}} \right] \)

Brightness = \( \frac{\text{Total flux}}{\text{solid angle} \cdot 0.1\% \text{ bandwidth}} \) \( \left[ \frac{\text{Photons/s}}{\text{mrad}^2 \cdot 0.1\% \text{ bandwidth}} \right] \)

Brilliance = \( \frac{\text{Total flux}}{\text{solid angle} \cdot \text{source area} \cdot 0.1\% \text{ bandwidth}} \) \( \left[ \frac{\text{Photons/s}}{\text{mrad}^2 \cdot \text{mm}^2 \cdot 0.1\% \text{ bandwidth}} \right] \)

Brilliance is the figure of merit for the design of new Synchrotron Radiation sources
Emission spectrum

- **Energie (eV):** 1 eV, 10 eV, 100 eV, 1 keV, 10 keV, 100 keV
- **Nombre de photons:** $10^{13}$, $10^{14}$, $10^9$, $10^{10}$, $10^{11}$, $10^0$
- **Longueur d'onde (Å):** $10^8$, $10^7$

**Graph:**
- **Phosphorescence:**
  - **X-ray tubes:**
  - **Bending magnet:**
  - **Sun**

**Data:**
- $\epsilon_e = 0.58$ KeV
- $E_e = 1.5$ GeV

**Legend:**
- **X-ray tubes**
- **Bending magnet**
- **Sun**
Magnetic wigglers and undulator (N periods)

Principle:
periodic arrangement of short bending magnets of alternating polarity perpendicular to the plane of the storage ring

Permanent magnetic materials e.g. Nd-Fe-B

⇒ force the electrons to oscillate („wiggle“) perpendicular to their direction of motion
⇒ Radiation is emitted during each individual wiggle
⇒ increase of the intensity
wiggler and undulator

\[ K := \alpha \cdot \gamma = \frac{eB_0 \lambda_0}{2\pi m_e c} \]

Wiggler regime: \( \alpha > 1/\gamma \)

Undulator regime: \( \alpha \sim 1/\gamma \)

In the undulator regime the radiation cones overlap and the wave trains can interfere.
Forms of Synchrotron Radiation

Bending magnet radiation

Wiggler radiation

Undulator radiation
Spectral Brightness

![Graph showing spectral brightness vs. photon energy for different sources like 1-2 GeV Undulators, 6-8 GeV Undulators, Wigglers, and Bending magnets.](image-url)
Examples of Wigglers and Undulators
Evolution of Brilliance

1st generation: Exploitation of the light from the bending magnets of e+/e- colliders originally built for elementary particle physics

2nd generation: Radiation from bending magnets and introduction of first insertion devices, lower e-beam emittance, optimization of light extraction

3rd generation: Dedicated storage rings, very low e-beam emittance, brilliance is figure of merit, mainly undulators, long straight sections
Evolution of Source Brilliance

Brilliance = \frac{\text{Spectral flux}}{\text{source area} \times \text{solid angle}}

Spring8

APS

ESRF

PETRA III under construction

Source size

3rd generation SRS

2nd generation SRS

1st generation SRS

X-ray tubes

1920 1940 1960 1980 2000

Year

10^6 10^9 10^{12} 10^{15} 10^{18}

Brilliance

Divergence
European Synchrotron Radiation Facility (ESRF)
Beamline organization

This is a typical x-ray beamline. Optics hutch contains elements for conditioning the x-ray beam.
How does a beamline work?
Basic principle of monochromator:
Bragg reflection from perfect single crystal

\[ 2d_{hk\ell} \sin \theta = n\lambda \]
Energy range of standard monochromator

Bragg Reflection

Si 111
Si 311
Si 511

Bragg angles

3°~27°

Energy range

4.4~110 keV

Photon energy (wavelength) can be selected by crystal, net planes, and Bragg angle.

Photon energy (wavelength) can be selected by crystal, net planes, and Bragg angle.
Double crystal monochromator

Problems with single crystal monochromators
- the monochromatic beam moves when the energy is changed
- high harmonic content
- big tails

Solution: double crystal design!
Simplest design: cutting a channel for the beam in a silicon block (channel cut monochromator)

- Use the same crystals and $d$-spacing for 1$^{\text{st}}$ and 2$^{\text{nd}}$ crystals
- Keep parallel setting
refractive index: $n = 1 - r_0 \rho \lambda^2 / 2\pi - i \mu \lambda / 4\pi$

By Snell’s law ($n_1 \cos(\theta_1) = n_2 \cos(\theta_2)$ with $\theta$ the grazing angle) in the absence of absorption (total reflection), we find total external reflection for angles less than $\theta_c \approx \lambda (r_0 \rho / \pi)^{1/2}$

$\theta_c$ typically a few mrad for x-ray mirrors

Surface roughness must be considered around critical energy (angle).
Bent mirrors (focusing and collimating)

Focusing of the x-ray beam → reflecting surface must have some curvature (achieved e.g. by bending mirror, **mirror focuses in one plane only!**)

Bending radius \( R \) (can be \(~ 10 \text{ km}\))

\[
R = \frac{2D_1D_2}{\theta(D_1 + D_2)}
\]

imaging the source in the vertical direction with unity magnification (1:1 focusing)

improving energy resolution of a following monochromator by production of a parallel beam (collimating)
Free electron laser (FEL)

Figure 1. Comparison of several recently commissioned FELs (FLASH and LCLS) and several planned FELs (sFLASH, Euro XFEL, NLS) with a state-of-the-art undulator beamline on the Diamond Light source. The standard definition of brightness is given in photons/unit time/unit solid angle/unit area/normalised bandwidth. Courtesy of STFC, New Light Source Conceptual Design Report (2010) [1].
SASE – spontaneous amplified self-emission

Linac-based Free Electron Laser
Self-Amplified Spontaneous Emission (SASE)

Principle design (SPring-8, Japan):

- e-gun (pulsed)
- linac (linear accelerator)
- undulator

Micro-bunching

X-Ray Laser

e-beam
Snapshots for different times after excitation ("pump-probe experiment") ⇒ “film” of the reaction
Obstacle: Coulomb-Explosion

Example:
Lysozyme
white: Hydrogen,
grey: Carbon,
blue: Nitrogen,
red: Oxygen,
yellow: Sulfur

Requirement: Pulse must be short enough and not to intense, to take picture before molecule disintegrates!

R. Neutze et al., Nature, August 2000
## Properties of vacuum

<table>
<thead>
<tr>
<th>Pressure (mbar)</th>
<th>Monolayer time constant (s)</th>
<th>Molecular density (m⁻³)</th>
<th>Mean free path (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00E+03</td>
<td>3E-09</td>
<td>2E+25</td>
<td>8E-09</td>
</tr>
<tr>
<td>1.00E+00</td>
<td>3E-06</td>
<td>2E+22</td>
<td>8E-06</td>
</tr>
<tr>
<td>1.00E-03</td>
<td>3E-03</td>
<td>2E+19</td>
<td>8E-03</td>
</tr>
<tr>
<td>1.00E-06</td>
<td>3E+00</td>
<td>2E+16</td>
<td>8E+00</td>
</tr>
<tr>
<td>1.00E-09</td>
<td>3E+03</td>
<td>2E+13</td>
<td>8E+03</td>
</tr>
<tr>
<td>1.00E-12</td>
<td>3E+06</td>
<td>2E+10</td>
<td>8E+06</td>
</tr>
<tr>
<td>1.00E-15</td>
<td>3E+09</td>
<td>2E+07</td>
<td>8E+09</td>
</tr>
</tbody>
</table>
Pressure regimes
Mean free path of electrons
Turbomolecular pump
Fig. I.7a,b. Schematic view of an ion-getter pump: (a) The basic multicell arrangement. Each cell consists essentially of a tube-like anode. The cells are sandwiched between two common cathode plates of Ti, possibly together with auxiliary cathodes of Ti. (b) Detailed representation of the processes occurring within a single cell. Residual gas molecules are hit by electrons spiralling around the magnetic field B and are ionized. The ions are accelerated to the cathode and/or auxiliary cathode; they are trapped on the active cathode surface or they sputter Ti atoms from the auxiliary cathode, which in turn help to trap further residual gas ions.
Vapor pressure

<table>
<thead>
<tr>
<th></th>
<th>$10^{-10}$ mbar</th>
<th>$10^{-6}$ mbar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>310K</td>
<td>400K</td>
</tr>
<tr>
<td>Zn</td>
<td>355K</td>
<td>450K</td>
</tr>
<tr>
<td>Cd</td>
<td>310K</td>
<td>390K</td>
</tr>
<tr>
<td>Hg</td>
<td>150K</td>
<td>230K</td>
</tr>
<tr>
<td>Mg</td>
<td>405K</td>
<td>505K</td>
</tr>
<tr>
<td>Al</td>
<td>860K</td>
<td>1100K</td>
</tr>
<tr>
<td>Fe</td>
<td>1000K</td>
<td>1300K</td>
</tr>
<tr>
<td>W</td>
<td>2160K</td>
<td>2680K</td>
</tr>
</tbody>
</table>
CF-flange
Ionization gauge
\[ \vec{E} = \vec{E}_0 e^{-\frac{k\omega}{c} \vec{n}_q \cdot \vec{r}} e^{i \left( \frac{n\omega}{c} \vec{n}_q \cdot \vec{r} - \omega t \right)} \]
Fig. 2.4 Frequency dependence of the real and imaginary parts of the complex dielectric constant of a dipole oscillator at frequencies close to resonance. The graphs are calculated for an oscillator with $\omega_0 = 10^{14}$ rad/s, $\gamma = 5 \times 10^{12}$ s$^{-1}$, $\epsilon_{st} = 12.1$, and $\epsilon_{\infty} = 10$. Also shown is the real and imaginary part of the refractive index calculated from the dielectric constant.
Fig. 3.14 Schematic diagram of the experimental arrangement required to determine the absorption coefficient over a wide spectral range by making reflectivity and transmissivity measurements.
Czerny-Turner monochromator
<table>
<thead>
<tr>
<th>Spectral region</th>
<th>Wavelength (nm)</th>
<th>Source</th>
<th>detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Infrared</td>
<td>&gt; 1600</td>
<td>Black body</td>
<td>Cooled semiconductor</td>
</tr>
<tr>
<td>Near infrared</td>
<td>700-1600</td>
<td>Black body</td>
<td>Semiconductor</td>
</tr>
<tr>
<td>Visible</td>
<td>400-700</td>
<td>Black Body</td>
<td>Photomultiplier</td>
</tr>
<tr>
<td>Ultraviolet</td>
<td>200-400</td>
<td>Xenon lamp</td>
<td>Photomultiplier</td>
</tr>
</tbody>
</table>
Spectral units

- Energie (eV)
- Frequenz (GHz)
- Wellenlänge (m)
- Wellenzahlen (cm$^{-1}$)

<table>
<thead>
<tr>
<th>Kurzwellen</th>
<th>Mikrowellen</th>
<th>Submm</th>
<th>Infrarot</th>
<th>VIS</th>
<th>UV</th>
</tr>
</thead>
</table>

- FIR
- MIR
- NIR

20 100 1000 10000 cm$^{-1}$
A black body's radiation
Photomultiplier

Figure 1

- Incoming Photon
- Photocathode
- Window
- Dynodes
- Anode
- Focusing Electrode
- Voltage Dropping Resistors
- Power Supply
- Output Meter

Photoelectron
Fourier-transform infrared spectrometer
5.1 When linearly polarized incident light, consisting of p- and s-orthogonal polarization components, is reflected from a surface at oblique angle of incidence ($\phi$) the result is often elliptical polarization. Ellipsometry measurements determine the change in polarization that occurs when light interacts with the sample.
Ellipsometry

\[ \rho = \frac{R_p}{R_s} = \tan \Psi \exp(i\Delta) \]
Optical conductivity

- complex dielectric constant: \( \epsilon = \epsilon_1 + i\epsilon_2 \)

- by definition: \( \sqrt{\epsilon} = n + ik = \hat{n} \)

\[
\begin{align*}
\epsilon_1 &= n^2 - k^2 \\
\epsilon_2 &= 2nk
\end{align*}
\]

- with complex conductivity: \( \sigma = \sigma_1 + i\sigma_2 \)

and \( \epsilon = 1 + \frac{i\sigma}{\epsilon_0\omega} \)

\[
\begin{align*}
\sigma_1 &= \epsilon_0 \epsilon_2 \omega \\
\sigma_2 &= \epsilon_0 (1 - \epsilon_1) \omega
\end{align*}
\]
<table>
<thead>
<tr>
<th></th>
<th>Dielectric constant ( \hat{\varepsilon} )</th>
<th>Conductivity ( \hat{\sigma} )</th>
<th>Refractive index ( \hat{N} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \hat{\varepsilon} )</td>
<td>( \hat{\varepsilon} = \varepsilon_1 + i\varepsilon_2 )</td>
<td>( \hat{\sigma} = \sigma_1 + i\sigma_2 )</td>
<td>( \hat{N} = n + ik )</td>
</tr>
<tr>
<td>( \sigma_1 )</td>
<td>( \sigma_1 = \frac{\omega\varepsilon_2}{4\pi} )</td>
<td>( \sigma_1 = \frac{nk\omega}{2\pi\mu_1} )</td>
<td>( \sigma_2 = \left(1 - \frac{n^2 - k^2}{\mu_1}\right)\frac{\omega}{4\pi} )</td>
</tr>
<tr>
<td>( \sigma_2 )</td>
<td>( \sigma_2 = (1 - \varepsilon_1)\frac{\omega}{4\pi} )</td>
<td>( \sigma_2 = \left(1 - \frac{n^2 - k^2}{\mu_1}\right)\frac{\omega}{4\pi} )</td>
<td>( \sigma_2 = \left(1 - \frac{n^2 - k^2}{\mu_1}\right)\frac{\omega}{4\pi} )</td>
</tr>
</tbody>
</table>

\[ n = \left\{ \frac{\mu_1}{2} \left[ \varepsilon_1^2 + \varepsilon_2^2 \right] \right\}^{1/2} + \frac{\varepsilon_1\mu_1}{2} \]

\[ k = \left\{ \frac{\mu_1}{2} \left[ \varepsilon_1^2 + \varepsilon_2^2 \right] \right\}^{1/2} - \frac{\varepsilon_1\mu_1}{2} \]

\[ n = \left\{ \frac{\mu_1}{2} \left[ \left(1 - \frac{4\pi\sigma_2}{\omega}\right)^2 + \left(\frac{4\pi\sigma_1}{\omega}\right)^2 \right] \right\}^{1/2} + \frac{\mu_1}{2} - \frac{2\pi\mu_1\sigma_2}{\omega} \]

\[ k = \left\{ \frac{\mu_1}{2} \left[ \left(1 - \frac{4\pi\sigma_2}{\omega}\right)^2 + \left(\frac{4\pi\sigma_1}{\omega}\right)^2 \right] \right\}^{1/2} - \frac{\mu_1}{2} + \frac{2\pi\mu_1\sigma_2}{\omega} \]
Table 7.1 Free electron density and plasma properties of some metals. The figures are for room temperature unless stated otherwise. The electron densities are based on data taken from Wyckoff (1963). The plasma frequency $\omega_p$ is calculated from eqn 7.6, and $\lambda_p$ is the wavelength corresponding to this frequency.

<table>
<thead>
<tr>
<th>Metal</th>
<th>Valency</th>
<th>$N$ $(10^{28} \text{ m}^{-3})$</th>
<th>$\omega_p/2\pi$ $(10^{15} \text{ Hz})$</th>
<th>$\lambda_p$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li (77 K)</td>
<td>1</td>
<td>4.70</td>
<td>1.95</td>
<td>154</td>
</tr>
<tr>
<td>Na (5 K)</td>
<td>1</td>
<td>2.65</td>
<td>1.46</td>
<td>205</td>
</tr>
<tr>
<td>K (5 K)</td>
<td>1</td>
<td>1.40</td>
<td>1.06</td>
<td>282</td>
</tr>
<tr>
<td>Rb (5 K)</td>
<td>1</td>
<td>1.15</td>
<td>0.96</td>
<td>312</td>
</tr>
<tr>
<td>Cs (5 K)</td>
<td>1</td>
<td>0.91</td>
<td>0.86</td>
<td>350</td>
</tr>
<tr>
<td>Cu</td>
<td>1</td>
<td>8.47</td>
<td>2.61</td>
<td>115</td>
</tr>
<tr>
<td>Ag</td>
<td>1</td>
<td>5.86</td>
<td>2.17</td>
<td>138</td>
</tr>
<tr>
<td>Au</td>
<td>1</td>
<td>5.90</td>
<td>2.18</td>
<td>138</td>
</tr>
<tr>
<td>Be</td>
<td>2</td>
<td>24.7</td>
<td>4.46</td>
<td>67</td>
</tr>
<tr>
<td>Mg</td>
<td>2</td>
<td>8.61</td>
<td>2.63</td>
<td>114</td>
</tr>
<tr>
<td>Ca</td>
<td>2</td>
<td>4.61</td>
<td>1.93</td>
<td>156</td>
</tr>
<tr>
<td>Al</td>
<td>3</td>
<td>18.1</td>
<td>3.82</td>
<td>79</td>
</tr>
</tbody>
</table>
Experimentelles Beispiel: Aluminium