X-ray spectroscopy

- Crystal spectrometers
- Reflection gratings
- Transmission gratings
- Solid state detectors
Bragg’s law

\[ n\lambda = 2d \sin \theta \]

This equation represents the Bragg’s Law, which describes the condition for constructive interference in X-ray crystallography. The diagram illustrates the concept, showing an incident plane wave interacting with a crystal structure, resulting in constructive interference when the condition specified by Bragg’s Law is met.
How are X-rays reflected from a surface?

- At short wavelengths, mirrors do not work well.
- Reflectivity of all materials becomes nearly zero at energies beyond 30 eV for normal incidence.
- At grazing incidence, reflectivity is maintained up to much higher energies.
- Spectrometers have to use as few reflections as possible.
How are X-rays reflected from a surface?

- Reflection of x rays from a surface is caused by the electrons which give it a refractive index \( n<1 \) at x ray wavelengths (solids have \( n>1 \) at optical wavelengths).
- X rays striking vacuum-metal interfaces are going from optically more-dense to optically less-dense media.
- In these circumstances total internal reflection of the light can occur.
- If the incidence angle is great enough (or the grazing angle is small enough) the X-rays are reflected from the surface.
- Value of the critical angle depends on the electron density of the mirror material. This number is particularly large for gold, platinum, iridium.

![Graph showing reflectivity of a gold mirror vs. photon energy (eV) for different incidence angles: 90°, 2°, 0.5°.](image)
Multilayer optics for x-rays

- Reflectivity of X-rays from a solid surface can be enhanced by using multilayers with nanometer spacing.
- Change of refractive index at each interface causes a partial reflection
- Interference effects enhance constructively total reflection efficiency

Reflectivity vs. Wavelength (nm)

Reflectivity is tailored to optimize a certain wavelength of interest
Multilayer optics for x-rays

- Curved mirror geometries are also possible
- X-ray analysis of chemical elements in microscopic samples
Crystal x-ray spectrometers

Some types:
- Von Hamos (cylindrical)
- Dumond (crystal in transmission)
- Johann (cylindrical)

High resolution spectra (up to R=20000) can be obtained.
The Rowland mounting

- Geometry suggested by Rowland in 1882.
- Combines the focusing properties of a spherical mirror with the diffraction properties of a grating.
- If a source and the grating are placed on a circle with half the radius $R$ of the grating, all wavelengths will be focused on the same circle: The Rowland circle.
Von Hamos crystal x-ray spectrometer

By bending crystals in sophisticated ways, focusing and imaging of x-ray sources can be achieved.
Transmission crystal x-ray spectrometer

- Dumond geometry: crystal works in transmission
- not affected by refractive index of crystal material
- application for hard x-rays, which are transmitted through crystal and partially reflected by many lattice layers
Johann x-ray spectrometer
The equivalence of mass and energy

The direct test of Einstein’s equation is based on the prediction that when a nucleus captures a neutron, the resulting isotope (mass number \(A+1\)) is somewhat lighter than the sum of the masses of the original nucleus (mass number \(A\)) and the free neutron (mass number 1). The energy equivalent to this mass difference is emitted as a spectra of gamma-rays.

The mass difference in Einstein’s equation using two silicon isotopes \(^{28-29}\text{Si}\) and two sulphur isotopes \(^{32-33}\text{S}\) has been measured with very high accuracy at the MIT, using a novel experimental technique.
The equivalence of mass and energy

The mass differences between the nuclei involved in the reaction are converted into photon energy. The masses are weighted in a Penning trap.

\[ \Delta Mc^2 = (M^{AX} - M^{A+1X} + M[D] - M[H])c^2 = 10^3 N_A h (f_{A+1} - f_D) \text{ mol AMU kg}^{-1} \] (1)

The photon energy is measured with the crystal spectrometer:

\[ f_{Si} = \frac{c}{(0.146318275(86) \times 10^{-12} \text{ m})} \]
\[ f_S = \frac{c}{(0.143472991(54) \times 10^{-12} \text{ m})} \]
\[ f_D = \frac{c}{(0.557341007(98) \times 10^{-12} \text{ m})} \]

The quantity \( 1-\Delta mc^2/E = (-1.4 \pm 4.4) \times 10^{-7} \) is obtained.

• Equivalence of mass and energy tested to a level of at least 0.00004%. 
The mass difference $\Delta m$ is measured by simultaneous comparisons of the cyclotron frequencies (inversely proportional to the mass) of ions of the initial and final isotopes confined over a period of weeks in a Penning trap. (S. Rainville et al., Science 2004)
The energies of the gamma-rays emitted after neutron capture by both silicon and sulphur have been measured at the using the world’s highest resolution gamma-ray interferometer GAMS4.

- Precision of better than 5 parts in 10,000,000.
High angular resolution is obtained by using high precision optical interferometers.

The crystals are mounted on interferometer arms which can be rotated in angular steps as small as 0.0004 arcsec (10^{-7}° or 2 \times 10^{-9} \text{ rad}).
Measurement of the 788 keV transition in $^{36}$Cl.
Data for testing E=mc²

a) Wavelength data and fitted curves. The energy of the emitted 5,421-keV γ-rays is measured from the angular separation of the second-order Bragg peaks resulting from diffraction from a silicon crystal.

b) Measured mass ratio $M^{[33S]} / M^{[32SH]}$ (which largely determines the mass change, m) as a function of the distance between the ions, s, in the Penning trap.

The final mass ratio (solid line) is determined with fractional accuracy of 7 parts in $10^{12}$ (dashed lines).

Flat crystal x-ray spectrometer

- Rail system
- Visible light entrance port
- Main chamber
- Crystal holder
- EBIT
- Beryllium window
- Camera port: transmission
- Camera port: reflection
- Camera
Absolute x-ray spectroscopy

A novel method removes the largest error sources found in crystal spectrometers.

Laboratory setup
Absolute measurements

\[ \Gamma = 180^\circ - 2\Theta \]

Bond method (W.L. Bond, Acta Cryst. 13, 814 (1960))
The Lyman-\(\alpha\) spectrum of hydrogenic Ar
Hydrogenic standards?

Current x-ray standards impaired by satellites

Calibration line
Fe Kα (1 ppm)

Best HCl line elsewhere
Ar$^{17+}$ Ly$\alpha_1$ (5 ppm)
The Lyman-alpha spectrum of hydrogenic Ar

\[ \sim 2 \text{ eV} \]
The Lyman-alpha spectrum of hydrogenic Ar
The He-like $S^{14+}$ spectrum

![Graph showing relative and absolute measurements for w-line $S^{14+}$ with Heidelberg EBIT and other data sources.]
Two-electron QED

Contributions to ground state in He-like $\text{Ar}^{16+}$

- Experimental error bar: $\approx \pm 0.01 \text{ eV}$
- Nuclear recoil: 0.06 eV
- Higher orders: 0.001 eV
Lamb shift in Li-like Bi$^{80+}$

Measurement of the Bi$^{80+}$ $2s_{1/2}-2p_{3/2}$ transition energy

Hyperfine splitting of the F=4, 5 levels

FIG. 1. Crystal spectrometer spectra obtained with a 100-keV, 170-mA electron beam: (a) $2s_{1/2}-2p_{3/2}$ transition in Li-like $^{209}$Bi$^{80+}$ showing the two components due to the $F = 4$ and $F = 5$ splitting of the ground state; (b) He-like C$^{15+}$ K-shell calibration spectrum. Lines $w$, $x$, $y$, and $z$ denote the transitions from upper levels $1s2p \, ^1P_1$, $1s2p \, ^3P_2$, $1s2p \, ^3P_1$, and $1s2s \, ^3S_1$, respectively, to the $1s^2 \, ^1S_0$ He-like ground level; lines $q$ and $r$ denote the transitions $1s2s2p \, ^2P_{3/2}$ and $1s2s2p \, ^2P_{1/2}$ to the $1s^2 2s \, ^2S_{1/2}$ Li-like ground level.
Lamb shift in Li-like $\text{Bi}^{80+}$

Hyperfine splitting of the F=4,5 levels

TABLE I. Contributions to the ground state hyperfine splitting of $\text{Bi}^{80+}$ and comparison with measurement (in eV).

<table>
<thead>
<tr>
<th>Contribution</th>
<th>Contribution Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point nucleus$^a$</td>
<td>+0.958</td>
</tr>
<tr>
<td>Finite charge distribution$^a$</td>
<td>$-0.111(2)$</td>
</tr>
<tr>
<td>Finite magnetization distribution$^a$</td>
<td>$-0.014(6)$</td>
</tr>
<tr>
<td>QED$^b$</td>
<td>$-0.003$</td>
</tr>
<tr>
<td>Electron correlations (Coulomb)$^a$</td>
<td>$-0.036$</td>
</tr>
<tr>
<td>Electron correlations (Breit)$^a$</td>
<td>+0.002</td>
</tr>
<tr>
<td>Electron correlations (finite size)$^a$</td>
<td>+0.004(2)</td>
</tr>
<tr>
<td>Total theory</td>
<td>0.800(7)</td>
</tr>
<tr>
<td>Experiment</td>
<td>0.820(26)</td>
</tr>
</tbody>
</table>

$^a$Reference [15].

$^b$Scaled value from Ref. [5].
Grazing incidence spectrometer
Reflection grating spectrum
Seya-Namioka VUV spectrometer

• The Seya-Namioka mounting is used at wavelengths > 30 nm for which reflectivity at normal incidence is still sufficient
• Special case of the Rowland mounting with an acceptable spectral resolution.
• It is widely used in plasma diagnostics and at synchrotrons.
• Height of grating structure has a strong effect on grating efficiency by imposing an additional diffraction condition
• The HETG gratings have a period of 0.2\(\mu\)m or 2000Å for the high-energy gratings, and 0.4\(\mu\)m or 4000Å, for the medium energy gratings.
• Gratings with 10000 grooves/mm (1000Å) are used already.
A pinhole transmission grating spectrometer

X-ray experiment with a two pinhole grating (a and b) spectrograph.
PFS: plasma focus x-ray source
C: capacitor for energy storage to feed discharge
SH: shutter
PH: pinhole to collimate x rays
PG: pinhole gratings

two spectra
Grazing incidence soft-x-ray spectrometer

• At wavelengths shorter than 30 nm, small grazing angles are needed.
• Detectors are mounted on the Rowland circle and moved under vacuum with bellows.
• Curved photographic plates and MCPs can also be used.

Figure 1  Layout of the spectrograph. A, slit; B, membrane; C, slit adjustment; D, diaphragms; E, grating; F, grating holder; G, vacuum by-pass; H, pivot slit and grating; I, mirror; J, access to zero order; K, pivot plate holder; L, plate holder support for vertical movement; M, plate holder; N, vertical movement drive; O, plate holder back; P, optical table; Q, diffusion pump; R, protecting screen; S, plate holder adjustment; T, grating adjustment; U, detachable valve; V, vacuum connections on by-pass; W, shutter; X, zero-order detector.
Grazing incidence imaging optics

• Kirkpatrick-Baez geometry uses two cylindrical x-ray mirrors at grazing incidence

• Each of the two cylindrical mirrors focuses in one coordinate.
Wolter telescope

- Grazing incidence mirror telescope for X-rays in satellites
- Uses concentric conic surfaces with a single common point
- Paraboloid-hyperboloid combination with two internal reflections.
After focusing by mirror, transmission or reflection gratings are used to add spectral dispersion when needed. This spectrograph produces images in individual wavelengths.
Chandra’s Wolter telescope
Spectral imaging with XMM and Chandra

Images of a supernova remnant at different soft x-ray wavelengths

Composite image
Space based x-ray telescopes

- Coronal Diagnostic Spectrometer (CDS) on SOHO (ESA/NASA Solar and Heliospheric Observatory)

- Two complementary systems; the Normal Incidence Spectrometer (NIS) and the Grazing Incidence Spectrometer (GIS).

Spectral range of operation
Diagnostics of fusion plasmas with VUV and x-rays

The diagnostic of temperature, density, plasma composition, radiative losses material transport in fusion reactors in tokamaks requires the use of many spectrometers.
The spectrum of hydrogen

- One needs three quantum numbers to define the state of a hydrogen (hydrogen-like) atom:
  - $n = 1, 2, 3...$ (principal)
  - $l = 0, ..., n-1$ (orbital)
  - $m = -l, ..., +l$ (magnetic)

- The energy depends only on the principal quantum number $n$.
  \[ E_n = -\frac{Z^2}{2n^2} \]

- i.e. in a non-relativistic theory the $(l,m)$ states are degenerate!

\[ \psi(r) = \psi(r, \theta, \varphi) = R_n(r) Y_{lm}(\theta, \varphi) \]

- The spectrum of hydrogen:
  - $1s$ $(n=1, l=0)$
  - $2s$ $(n=2, l=0)$
  - $2p$ $(n=2, l=1)$
  - $3s$ $(n=3, l=0)$
  - $3p$ $(n=3, l=1)$
  - $3d$ $(n=3, l=2)$

Energy (au)

- Free electron
  - $-1/2$

- Bound electron
  - $-1/18$
  - $-1/8$

- $\ldots$
Dirac theory

\[ E_{nj} = mc^2 \sqrt{1 + \left( \frac{Z\alpha}{n - |j + 1/2| + \sqrt{(j + 1/2)^2 - (Z\alpha)^2}} \right)^2} \]

- **Positive continuum**
- **Negative energy continuum**

**bound states**

- \( n \): principle quantum number
- \( j \): total angular momentum
- \( \alpha \): fine structure constant - \( \alpha = 1/137.036 \)

\( mc^2 \): electron rest mass (511 keV)

**Dirac-Theorie:** (complete relativistic treatment of single electron systems)

*All levels with the same \( n \) and \( j \) are degenerate.*
**The Lamb shift**

- **Experiment:** Lamb-Retherford 1947;
- **Theoretical Explanation:** Bethe 1947
- **Experiment proves that** $2s_{1/2}$ and $2p_{1/2}$ **are not degenerate**
- **Contradicts Dirac theory**

Lamb shift (LS) includes all deviations from the Dirac theory for a point like nucleus

Consequence of the interaction of the bound electron with its own radiation field (self energy).
• The effects of QED on the binding energy increase with the strength of the electric field.
• s electrons are most affected since their .

\textit{Lamb shift (three effects)}

• Self-energy
• Vacuum polarization
• Size of the nucleus
Laser spectroscopy of hydrogen
Lamb shift: An effect of strong fields

- QED corrections to binding energy $\Delta E$ scale as:

  $$\Delta E \sim \frac{Z^4}{n^3}$$

  $Z$: nuclear charge
  $n$: principal quantum number

- Probability density in the region of highest field gradients is essential
Average field strength of 1s electron

\[ \langle E \rangle \ (V/cm) \]

Nuclear charge \( Z \)

The graph shows how the average field strength \( \langle E \rangle \) changes by six orders of magnitude from H atom to H-like U\(^{91+}\) as the nuclear charge \( Z \) increases.
Self energy (SE)

Self-energy: Describes the emission and reabsorption of a virtual photon (Bethe 1947) *The self energy decreases the binding energy.*

- The self-energy decreases the binding energy. Classical theory: infinitely high mass corresponding to an infinitely high self energy.
- First calculations for H were made by Bethe based on an idea of Kramer: mass renormalization. The interaction with virtual photon modifies the electron mass.
- Measured electron mass \(m\) already includes this radiation correction. \(\partial m\)
- The self-energy correction for a bound state is equivalent to mass difference between the bound electron and a non-interacting free electron of the mass \(m_e\).
Vacuum Polarization (VP)

- Virtual creation and annihilation of an $e^+e^-$ pair
- VP acts attractive
Summary of Lamb shift contributions

\[ \Delta E = \frac{\alpha}{\pi} (\alpha Z)^4 F(\alpha Z) \, m_e c^2 \]

- Self energy
- Vacuum polarization

**Individual corrections in detail**

<table>
<thead>
<tr>
<th></th>
<th>Hydrogen, H</th>
<th>H-like uranium, U^{91+}</th>
</tr>
</thead>
<tbody>
<tr>
<td>2p_{1/2} \rightarrow 1s_1</td>
<td>10.2 eV</td>
<td>97.6 keV</td>
</tr>
<tr>
<td>\text{Fine structure}</td>
<td>45.4 \mu eV</td>
<td>4.56 keV</td>
</tr>
<tr>
<td>2sLS</td>
<td>4.4 \mu eV</td>
<td>75.3 eV</td>
</tr>
<tr>
<td>1sLS</td>
<td>35.6 \mu eV</td>
<td>463.95 eV</td>
</tr>
</tbody>
</table>

**Plot**

- 1s Lamb Shift, \( \Delta E / Z^4 \) [meV]
- Nuclear charge number, Z
Bound-State QED: 1s Lamb Shift at High-Z

Sum of all corrections, leading to deviations from the Dirac theory for a point-like nucleus

**Self energy**

- $U^{92+}$
- $355.0 \text{ eV}$

**Vacuum polarization**

- $\Delta E = \frac{\alpha}{\pi} (\alpha Z)^4 F(\alpha Z) m_e c^2$
- $\alpha Z \ll 1$
- $F(\alpha Z)$: series expansion in $\alpha Z$

- $\alpha Z \approx 1$
- $F(\alpha Z)$: series expansion in $\alpha Z$
- Not appropriate

**Goal:** $\pm 1 \text{ eV}$
QED correction in second order $\alpha$

SE – SE

VP – VP

SE – VP

S(VP)E
GSI accelerator gacility

UNILAC
11.4 MeV/u
U^{73+}

ESR
10 - 500 MeV/u
U^{92+}

SIS
up to 1000 MeV/u
U^{92+}
Operation parameters
\( v/c = \beta \approx 0.65 \)

Revolution frequency
\( f \approx 10^6 \text{ s}^{-1} \)

Circumference: 108 m
Number of ions: \(10^8\)

Production of characteristic x-rays by electron capture into bare ions (electron cooler or jet-target)

Storage rings for heavy ions

ESR (GSI, Darmstadt)
Storage rings: cooled ion beams

- Electron collector
- Electron gun
- High voltage platform
- Magnetic field
- Electron beam
- Ion beam

Storage rings: cooled ion beams
Ions interact $10^6$ times per second with a collinear beam of cold electrons at nearly the same speed: cooling in the cold electron bath. → The transversal components of the ion motion are efficiently cooled.

Properties of the cold ions:
Momentum spread $\Delta p/p : 10^{-4} – 10^{-5}$
Beam diameter 2 mm

Electron cooling in storage rings

I: 5-500 mA
U: 10 - 200 kV
The effect of cooling

Ions interact $10^6$ times per second with collinear beam of cold electrons

Properties of the cold ion beam

- Momentum spread $\Delta p/p : 10^{-4} – 10^{-5}$
- Beam diameter 2 mm
Merged-beams kinematics

- Provides precise access to low relative collision energies

Relative energy, $E_{\text{rel}}$ (eV) vs. Electron energy, $E_{\text{e}}$ (eV)

- $E_{\text{cool}} = \frac{m_{\text{e}}}{m_{\text{ion}}} E_{\text{ion}}$
- Relative velocity: $v_{\text{rel}} = |v_{\text{e}} - v_{\text{ion}}|$
- Relative energy: $E_{\text{rel}} = (\sqrt{E_{\text{e}}} - \sqrt{E_{\text{cool}}})^2$
The GSI Electron Cooler

Electron Cooler

- 2.5 m interaction zone
- Voltage: 5 to 200 kV
- Current: 10 to 1000 mA
Dielectronic recombination: SR technique

merged-beams rate coefficient: $\alpha = \langle \sigma v \rangle$

$U_{\text{cath}}$
Doppler correction: Strong dependence on the velocity and the observation angle $\theta_{\text{LAB}}$

$$\gamma = \frac{1}{\sqrt{1 - \beta^2}}; \quad \beta = \frac{v}{c}$$

Relativistic Doppler transformation

$$E_{\text{lab}} = \frac{E_{\text{proj}}}{\gamma \cdot (1 - \beta \cdot \cos \theta_{\text{lab}})}$$

$E_{\text{lab}}$: Photon energy in the laboratory system
$E_{\text{proj}}$: Photon energy in the emitter system

Experimental challenges
Excited states are produced by electron capture (gas jet target) / recombination (electron target)
Blue shift has its maximum \( \beta \approx 0.29 \Rightarrow E_{\text{lab}} \approx 1.43 \times E_{\text{proj}} \)

\( \Delta \theta_{\text{LAB}} \) not critical, almost no Doppler width

Uncertainty caused by \( \Delta \beta \) has its maximum

Coincidence with the “downcharged” projectile (U\(^{91+}\)) reduces background
Ground state Lamb shift in H-like uranium

1s Lamb shift in U$^{91+}$

460.2$\pm$2.3$\pm$3.5 eV

4.6 eV

statistical uncertainty in $\beta$
Ground state Lamb shift in H-like uranium

Presently most accurate test of the bound-state QED for one-electron systems in the regime of strong fields carried out at the ESR.
Test of quantum electrodynamics

1s Lamb shift in H-like uranium

Experiment: 459.8 eV ± 4.6 eV
Theory: 463.95 eV

A. Gumberidze
PhD thesis 2003,
PRL 94, 223001 (2005)