X-ray sources and optics

Dimosthenis Sokaras

SLAC National Accelerator Laboratory
Electromagnetic Waves Spectrum: X-rays

Energy $\rightarrow$ 0.1-100keV

Wavelength $\rightarrow \lambda[\text{Å}] = \frac{12.398}{E[\text{keV}]} \rightarrow 0.1 - 60\text{Å}$
Properties for the interaction of X-ray with matter are theoretically described with this Hamiltonian interaction:

\[ H = H_0 - \frac{e}{mc} \mathbf{p} \cdot \mathbf{A}(\mathbf{r}) + \frac{1}{2m} \left( \frac{e}{c} \right)^2 \mathbf{A}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \]

- absorption/emission
- scattering
X-ray Sources: Motivation – Aim in Research

\[ E\Psi(r) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + V(r)\Psi(r) \]
Main Mechanisms for X-ray Sources

- **Characteristic X-rays**
  - Relaxation of atomic excited states

- **Acceleration of charged particles**
  - Synchrotron Radiation
  - Bremsstrahlung Radiation
  - Plasma sources
Properties for an X-ray source

Performance Properties
- energy content
- flux
- Beam size
- angular convergence
- stability
- polarization
- time domain
- Coherence

Practical Properties
- Cost
- Availability/Access
- Portability

\[ \text{Flux} = \frac{\text{# of photons in given } \Delta \lambda / \lambda}{\text{sec}} \]

\[ \text{Brightness} = \frac{\text{# of photons in given } \Delta \lambda / \lambda}{\text{sec, mrad } \theta, \text{ mrad } \phi, \text{ mm}^2} \] (a measure of concentration of the radiation)

\[ \text{Brightness} = \text{constant} \times \frac{F}{S \times \Omega} \]
Characteristic X-rays based Sources:

- Ionization of Primary Targets by means of irradiation:
  - Heavy ions (Electrostatic Accelerators)
  - Electrons (X-ray Tubes, e\(^-\) accelerators)
X-ray Sources: X-ray Tubes

Characteristic X-rays based Sources:

- X-ray Tubes
  - 1% of power becomes x-rays
  - Limitation = heat of the anode
  - Few W to several kW
  - Few to tens of keV photons
  - $4\pi$ emission
X-ray Sources: X-ray Tubes

Characteristic X-rays based Sources:

- X-ray Tubes
  - Fixed anode tube
  - Rotating Anode
  - Liquid Metal Anode
### Characteristic X-rays based Sources:

#### X-ray Tubes

**Table 1**  
Approximate X-ray beam brilliance for the main types of in-house sources with optics.

<table>
<thead>
<tr>
<th>System</th>
<th>Power (W)</th>
<th>Actual spot on anode (µm)</th>
<th>Apparent spot on anode (µm)</th>
<th>Brilliance (photons s⁻¹ mm⁻² mrad⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard sealed tube</td>
<td>2000</td>
<td>10000 × 1000</td>
<td>1000 × 1000</td>
<td>0.1 × 10⁹</td>
</tr>
<tr>
<td>Standard rotating-anode generator</td>
<td>3000</td>
<td>3000 × 300</td>
<td>300 × 300</td>
<td>0.6 × 10⁹</td>
</tr>
<tr>
<td>Microfocus sealed tube</td>
<td>50</td>
<td>150 × 30</td>
<td>30 × 30</td>
<td>2.0 × 10⁹</td>
</tr>
<tr>
<td>Microfocus rotating-anode generator</td>
<td>1200</td>
<td>700 × 70</td>
<td>70 × 70</td>
<td>6.0 × 10⁹</td>
</tr>
<tr>
<td>State-of-the-art microfocus rotating-anode generator</td>
<td>2500</td>
<td>800 × 80</td>
<td>80 × 80</td>
<td>12 × 10⁹</td>
</tr>
<tr>
<td>Excilium JXS-D1-200</td>
<td>200</td>
<td>20 × 20</td>
<td>20 × 20</td>
<td>26 × 10⁹</td>
</tr>
</tbody>
</table>

X-ray Sources: Synchrotron Radiation

Synchrotron Radiation based Sources

- **Storage Rings**
  - Large Scale Laboratories
  - Relativistic Electrons/Positrons (1-7 GeV)
  - Acceleration Magnetic Field
  - Insertion Devices
  - Emission cone in forward angles
X-ray Sources: Synchrotron Radiation

Synchrotron Radiation based Sources:

- **Storage Rings**
  - Bending Magnets ($\sim 10^{11}$ photons/s)
  - Wigglers ($\sim 10^{13}$ photons/s)
  - Undulators ($\sim 10^{14}$ photons/s)

- **Properties**
  - Unprecedented flux
  - Very broad energy range
  - Forward emission / small divergence
  - Polarization
X-ray Sources: Synchrotron Radiation

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Graph showing flux vs. energy for different Synchrotron Radiations:

- BL12
- BL6
- BL4
- BL14

SSRL, T. Rabedeau
X-ray Sources: X-ray Free Electron Laser

**Undulator**

Uncorrelated electron positions / radiated fields

**Very long Undulator - XFEL**

Microbunching by own radiated fields strongly correlated waves of electron and fields

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**X-ray Free Electron Laser**

- Undulator
  - Uncorrelated electron positions / radiated fields
- **Very long Undulator - XFEL**
  - Microbunching by own radiated fields strongly correlated waves of electron and fields

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**Graph**

- **E [J]**
  - **z [m]**
  - Courtesy of K-J. Kim

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**Diagram**

- **Undulator**
  - Magnetic field configuration
  - Uncorrelated electron positions
  - Radiated fields
- **Very long Undulator - XFEL**
  - Magnetic field configuration
  - Microbunching by own radiated fields
  - Strongly correlated waves of electron and fields
First lasing and operation of an angstrom-wavelength free-electron laser

P. Emma1,*, R. Akre1, J. Arthur1, R. Bionta2, C. Bostedt1, J. Bozek1, A. Brachmann1, P. Bucksbaum1, R. Coffee1, F.-J. Decker1, Y. Ding1, D. Dowell1, S. Edstrom1, A. Fisher1, J. Frisch1, S. Gilevich1, J. Hastings1, G. Hays1, Ph. Hering1, Z. Huang1, R. Iverson1, H. Loos1, M. Messerschmidt1, A. Miahnahri1, S. Moeller1, H.-D. Nuhn1, G. Pile3, D. Ratner1, J. Rzepiela1, D. Schultz1, T. Smith1, P. Stefan1, H. Tompkins1, J. Turner1, J. Welch1, W. White1, J. Wu1, G. Yocky1 and J. Galayda1

The recently commissioned Linac Coherent Light Source is an X-ray free-electron laser at the SLAC National Accelerator Laboratory. It produces coherent soft and hard X-rays with peak brightness nearly ten orders of magnitude beyond conventional synchrotron sources and a range of pulse durations from 500 to <10 fs (10^-15 s). With these beam characteristics this light source is capable of imaging the structure and dynamics of matter at atomic size and timescales. The facility is now operating at X-ray wavelengths from 22 to 1.2 Å and is presently delivering this high-brilliance beam to a growing array of scientific researchers. We describe the operation and performance of this new ‘fourth-generation light source’.

Figure 4 | FEL gain length measurement at 1.5 Å. Measured FEL power (red points) plotted after continuous insertion of each 3.4-m undulator segment showing saturation at 60 m and with all 33 undulator segments installed. Error bars represent the r.m.s. statistical uncertainty in the measured power when averaging 30 beam pulses. The measured gain length is 3.5 m with a GENESIS simulation overlaid (blue curve) and with consistent electron beam parameters shown. The YAG screen image is shown in the inset with 140-μm r.m.s. round X-ray spot size in this early case (April 2009). λ, is the fundamental FEL radiation wavelength; I0, is the peak current of the electron beam in the undulator; γ is the relativistic Lorentz factor; κx, is the transverse r.m.s. emittance of the electron beam in the undulator; κx, is the normalized transverse r.m.s. emittance of the electron beam in the undulator; σr/E0 is the r.m.s. relative energy spread of the electron beam in the undulator (that is, the r.m.s. energy spread, σr, divided by the mean electron energy, E0).

1SLAC National Accelerator Laboratory, Stanford, California 94309, USA, 2Lawrence Livermore National Laboratory, Livermore, California 94550, USA, 3Argonne National Laboratory, Argonne, Illinois 60439, USA. *e-mail: emma@slac.stanford.edu
Quality Factor for X-ray Sources

**Brilliance** = Radiated power per unit area per unit solid angle per unit spectral bandwidth

Unit → photons/s/mrad$^2$/mm$^2$/0.1%bandwith

Brilliance → Invariant quantity
X-ray Sources: Brilliance

X-ray tubes

Synchrotron Radiation sources

X-ray FELs
Natural X-ray Sources:

- Radioisotopes ($^{241}$Am, $^{55}$Fe, $^{109}$Cd, etc.)
- Stars, Super Novas, Cosmic Background

An X-ray image of the Sun, $T \sim 2 \cdot 10^6 K$
X-ray Sources: Motivation – Aim in Research

\[ E\Psi(r) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + V(r)\Psi(r) \]
Transferring x-ray photons (beam) to the sample:

- focus size
- energy content
- angular convergence
- stability
- polarization

The job of x-ray optics is to transform the source beam characteristics to provide the best possible match to the sample requirements.
X-ray Optics: Principles

X-rays Interaction Mechanisms for Optics:

- X-ray Diffraction (monochromatizing x-rays)
- X-ray Refraction/Reflection (guiding/collimating)
X-ray Optics: Refractive Index

Refractive index  \[ n = \frac{c}{u_p} \]

\[ n = 1 - \delta + i\beta \]

attenuation term

phase term
X-ray Optics: Refraction

Refraction

Snell Law: \[ \sin \phi' = \frac{\sin \phi}{n} \]

\( n < 1 \)  \( \Rightarrow \)  \( \phi' > \phi \)
Total external reflection

\[ n \approx 1 - \delta \implies \cos \vartheta_c = 1 - \delta \implies \vartheta_c = \sqrt{2\delta} \implies \vartheta_c \propto n \sqrt{Z} \]

\[ \delta \sim 10^{-5}-10^{-6} \implies \theta_c < 3^\circ-4^\circ \]
X-ray Optics: X-ray Mirrors

**Focusing**
condense beam to source dimensions on sample
demagnify source image to better couple photons on small sample at the expense of greater angular convergence on sample)

**Collimation**
collimate divergent beam to improve energy resolution of a monochromator

**Power filter**
absorb waste power at low power density on grazing incident optic

**Harmonic filter**
suppress higher energy contamination of beam (low pass filter)
X-ray Optics: X-ray Mirrors

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Collimation
\textit{collimate} energy resolution of a monochromator.

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The Kirkpatrick-Baez mirror system

(Courtesy of J. Underwood)
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Reflectivity

Energy (keV)

Si
Rh
Pt

2.7 mrad alpha
**Bragg Diffraction:** Constructive interference of radiation reflections from sequential planes.

\[ m\lambda = 2d \sin(\theta) \]
X-ray Optics: X-ray Diffraction

• Diffraction Gratings

\[ m \frac{\lambda}{d} = (\sin \alpha + \sin \beta) \]

soft x-rays

• Bragg-type x-ray crystal optics

\[ 2d_{hkl} \sin \theta = \lambda \]

hard x-rays
Energy Resolution - Darwin width (dynamical diffraction theory) and geometrical factors

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

\[ \frac{\lambda}{\Delta \lambda} = \frac{\tan \theta}{\Delta \theta} \]

Darwin width curves

65 meV @ 6462 eV

Darwin width for Si(440) @ 88 deg
X-ray Optics: Double Crystal monochromators

Liquid Nitrogen Cooled Monochromators

cooling channel bundle
X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram

T. Rabedeau, SSRL
X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram

T. Rabedeau, SSRL
X-ray Optics: Double Crystal Monochromators - Dupond and Acceptance Diagram

energy resolution:
- Darwin = 32.4
- total = 64.7

beam convergence/divergence

T. Rabedeau, SSRL
Doubly Curved Crystals

- Based on Bragg Diffraction
- Monochromator & Focusing

Curved vs. Plate Crystal

- Increased beam area that meets Bragg condition.
- Improve Energy resolution
- Focusing Effect

Rowland circle

Source

Focus

2R
X-ray Optics: Monochromatizing Divergent Sources
X-ray Optics: X-rays transmission in waveguides

Analytical description of waveguide

\[ f(x, y, z) = \left( \sqrt{x^2 + y^2} - R \right)^2 + z^2 - r^2 = 0 \]

Angle of incidence at point \( A(x,y,z) \)

\[ \vartheta = \sin^{-1}(l_0 \cdot n) \]

Angle of incidence at \( B(2\sqrt{rR}, R - r, 0) \)

\[ \sin \vartheta_{\text{max}} = \frac{2 \sqrt{rR}}{R + r} \]

Geometrical Parameters constrain

\[ \frac{R \vartheta_c^2}{4r} > 1 \]
X-ray Optics: X-rays transmission in waveguides

Reflectivity

\[ R_\phi = \frac{\left| \frac{\phi - \sqrt{(\phi^2 - \phi_c^2) + 2i\beta}}{\phi + \sqrt{(\phi^2 - \phi_c^2) + 2i\beta}} \right|^2}{\left| \frac{\phi - \sqrt{(\phi^2 - \phi_c^2) - 2i\beta}}{\phi + \sqrt{(\phi^2 - \phi_c^2) - 2i\beta}} \right|^2} \]

Photon energy: 8 keV
Bundles of thousands glass mono-capillaries in certain arrangements can be used for:

- Directing
- Focusing
- Parallelizing
X-ray Optics: Polycapillary X-ray lenses
## Polycapillary lens

**Functionality:** Spot focusing of diverging x-ray beam.

**Main Applications:** Focusing x-ray tubes beams.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_1, d_2$</td>
<td>0.3...1 mm</td>
</tr>
<tr>
<td>$d_{\text{max}}$</td>
<td>1...2 mm</td>
</tr>
<tr>
<td>$l$</td>
<td>40...50 mm</td>
</tr>
<tr>
<td>$f_1, f_2$</td>
<td>15...100 mm</td>
</tr>
<tr>
<td>FWHM</td>
<td>15...100 $\mu$m</td>
</tr>
</tbody>
</table>
X-ray Optics: Polycapillary-based XRF

X-ray tube based Micro-XRF setup
Summary

X-ray Sources
  X-ray Tubes
  Synchrotron Radiation Beamlines

X-ray Optics
  Mirrors
  Monochromators

  Double Curved Crystals
  Polycapillary lenses
Thank you!