國家同步輻射研究中心
National Synchrotron Radiation Research Center

同步輻射在X光繞射上的應用
Applications of Synchrotron Radiation in X-ray Diffraction

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南一中演講

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大綱

Synchrotron radiation（同步輻射）

- History and general background (背景說明)
- Properties (特性)
- Sources (bend magnets, wigglers, undulators) (光源)

X-ray diffraction (X光繞射)

- History and general background (背景說明)
- Basics of crystal structure (晶體結構)

Applications (應用)

- Material science (材料科學)
- Protein structure (大分子結構)
- X-ray cavity (X光共振腔--X光繞射實驗)

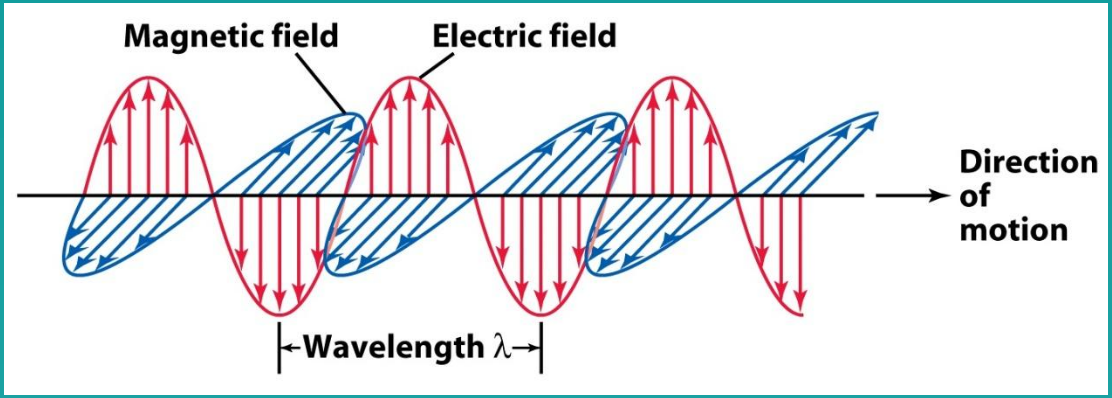
TPS project (台灣光子源計畫)

同步輻射
Synchrotron Radiation

James Clerk Maxwell 馬克斯威爾

Light is a traveling electromagnetic wave (1862)

- Unified electromagnetism and optics
- Predicted the existence of invisible forms of light

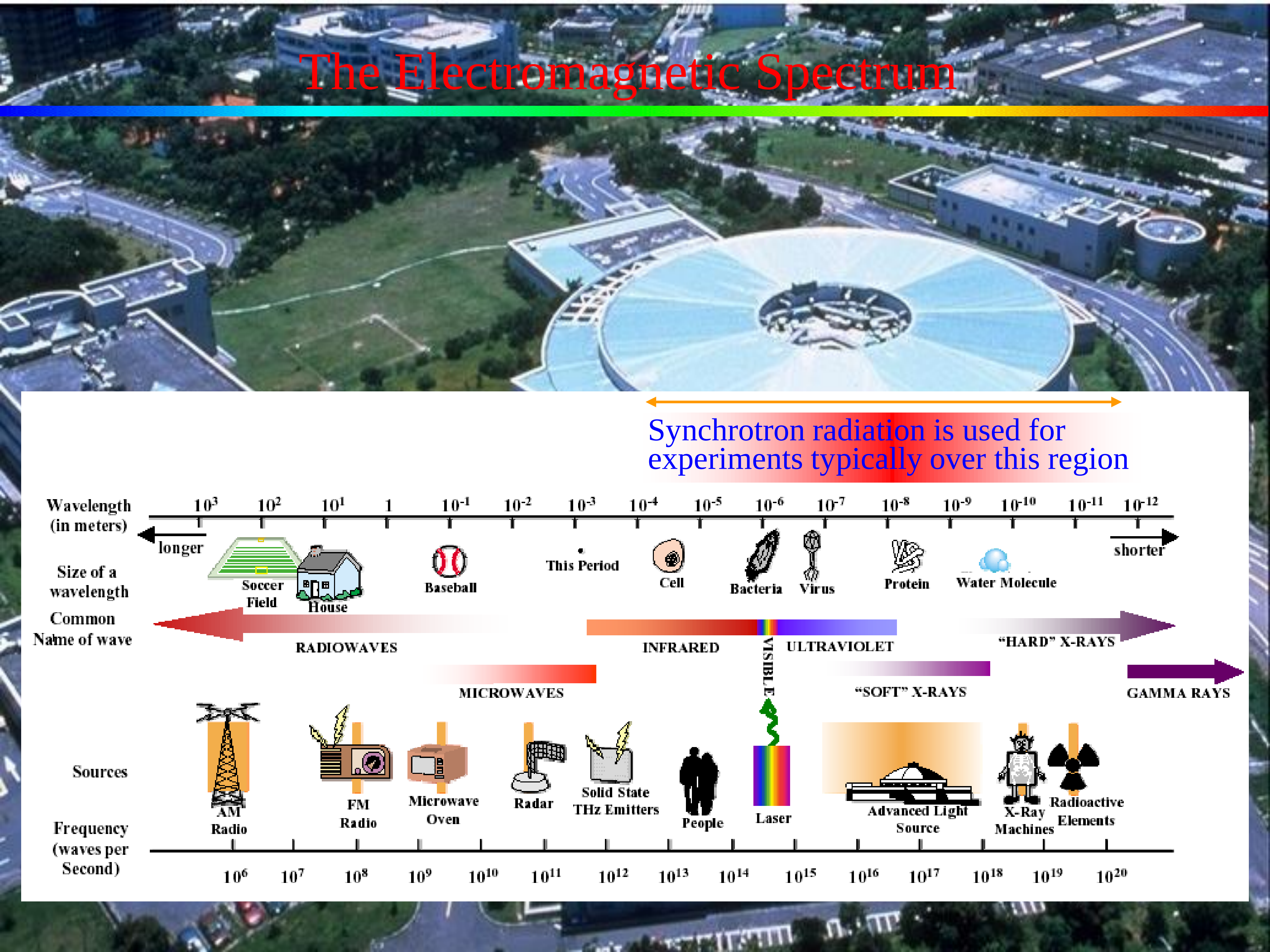


(1831-1879)
Scottish

Maxwell equation

$$\nabla \cdot E = \frac{\rho}{\varepsilon} \qquad \nabla \cdot B = 0$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \qquad \nabla \times B = \mu J + \varepsilon\mu \frac{\partial E}{\partial t}$$



The Electromagnetic Spectrum
Synchrotron radiation is used for
experiments typically over this region
Wavelength (in meters)
10³ 10² 10¹ 1 10⁻¹ 10⁻² 10⁻³ 10⁻⁴ 10⁻⁵ 10⁻⁶ 10⁻⁷ 10⁻⁸ 10⁻⁹ 10⁻¹⁰ 10⁻¹¹ 10⁻¹²
longer
shorter
Size of a wavelength
Soccer Field
House
Baseball
This Period
Cell
Bacteria
Virus
Protein
Water Molecule
Common Name of wave
RADIOWAVES
INFRARED
VISIBLE
ULTRAVIOLET
"HARD" X-RAYS
MICROWAVES
"SOFT" X-RAYS
GAMMA RAYS
Sources
AM Radio
FM Radio
Microwave Oven
Radar
Solid State THz Emitters
People
Laser
Advanced Light Source
X-Ray Machines
Radioactive Elements
Frequency (waves per Second)
10⁶ 10⁷ 10⁸ 10⁹ 10¹⁰ 10¹¹ 10¹² 10¹³ 10¹⁴ 10¹⁵ 10¹⁶ 10¹⁷ 10¹⁸ 10¹⁹ 10²⁰

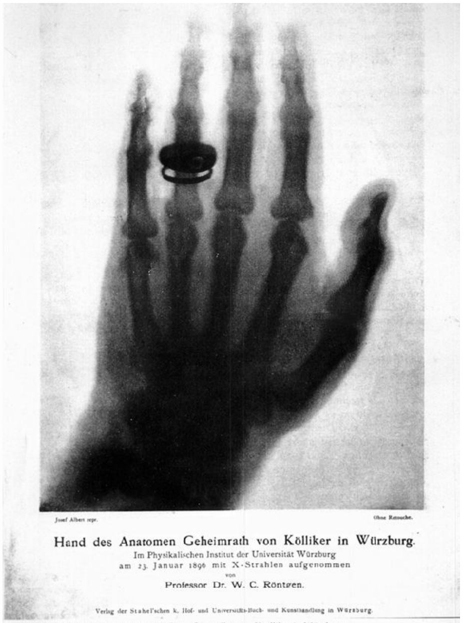
Discovery of X-rays

The Nobel Prize in physics in 1901

"in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him"

Wilhelm Conrad Röntgen

Germany (1845-1923)



Radiograph of the hand of the anatomist Privy Councillor von Koelliker in Würzburg, taken by W. C. Röntgen in Würzburg on January 23, 1896

Röntgen used photographs of his wife's hand to publicize his discovery.

They appeared in newspapers of the time and captured the publics imagination.

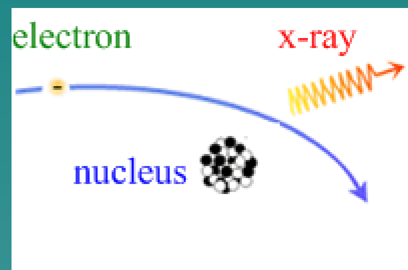
Roentgen's Laboratory in Wurzburg, Germany

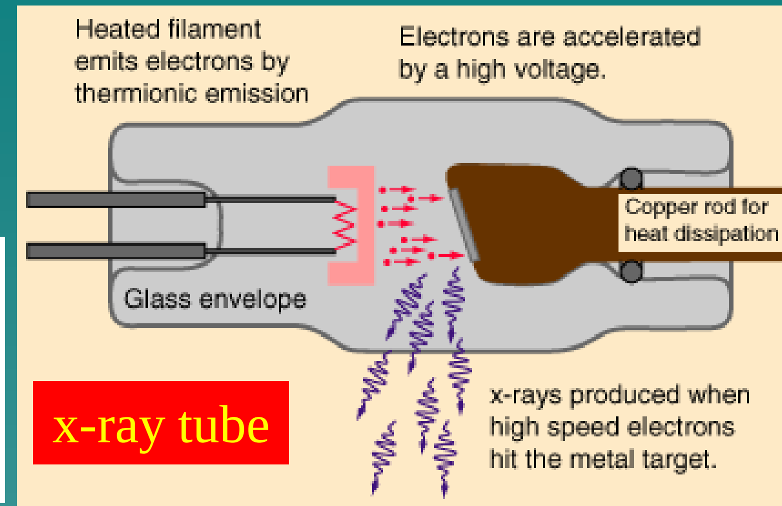
Röntgen performed experiments with cathode rays (electron beams) in 1895.

How to Generate X-rays

1. Bremsstrahlung (braking radiation)

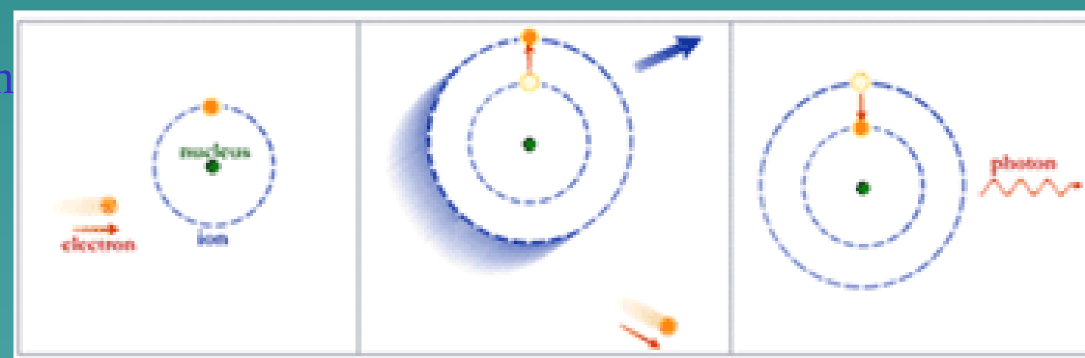
- electrons from an external source are deflected around the nucleus of an atom
- various wavelengths





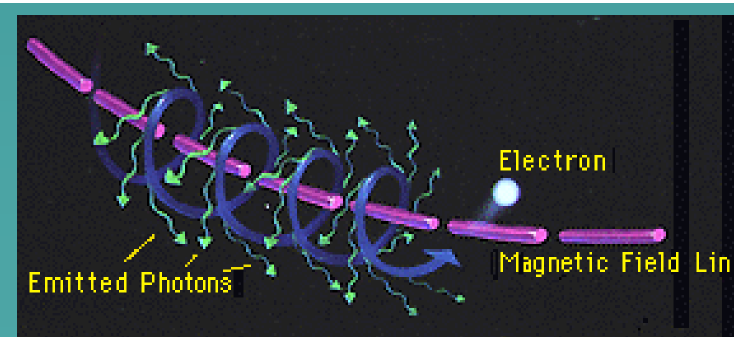
2. K-shell emission

- electrons change orbits within atom
- higher-intensity x-rays than bremsstrahlung, and a single wavelength.



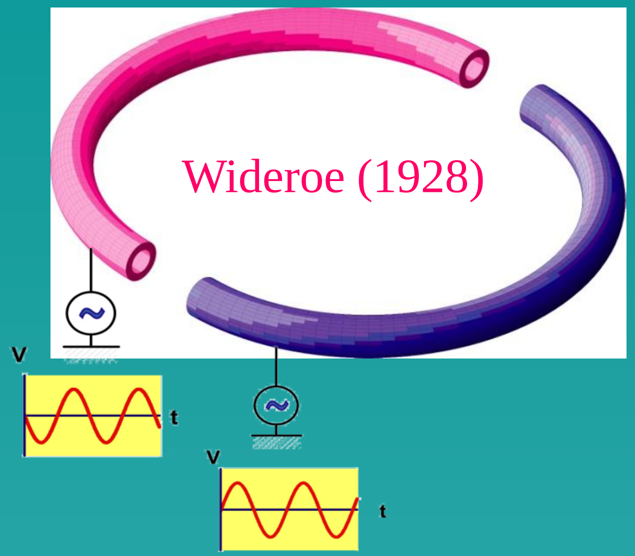
3. Accelerator: Synchrotron

Relativistic electron spirals around a magnetic field line

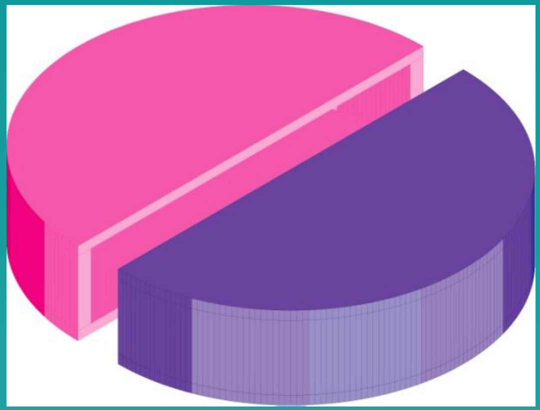


From Wideroe linac to cyclotron and synchrotron

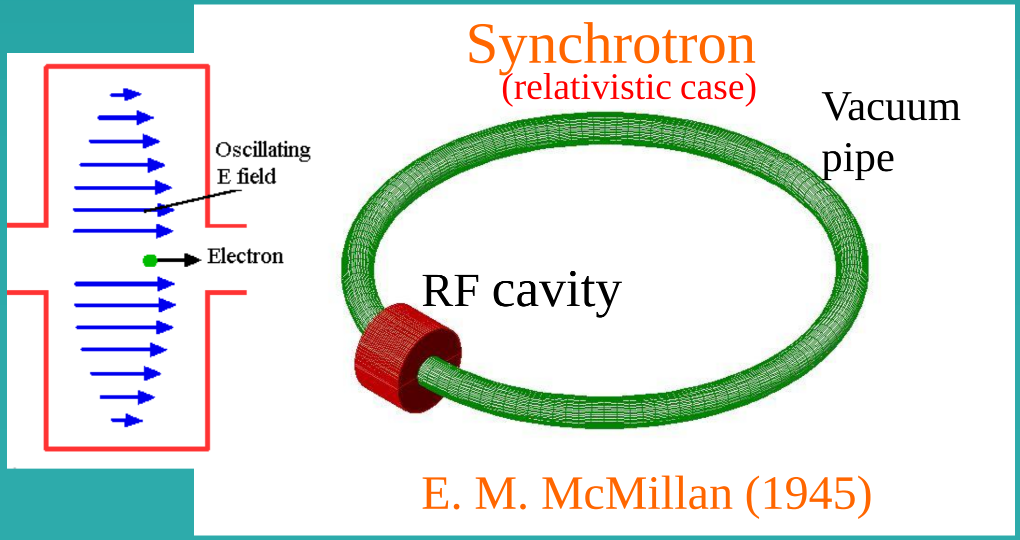
Alternating current Accelerator



Cyclotron (non-relativistic case)



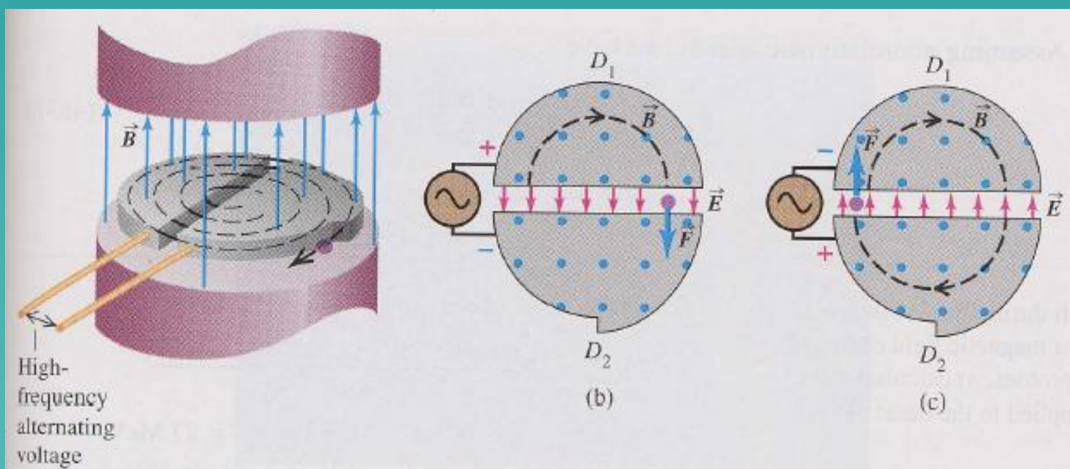
E. O. Lawrence (1932)

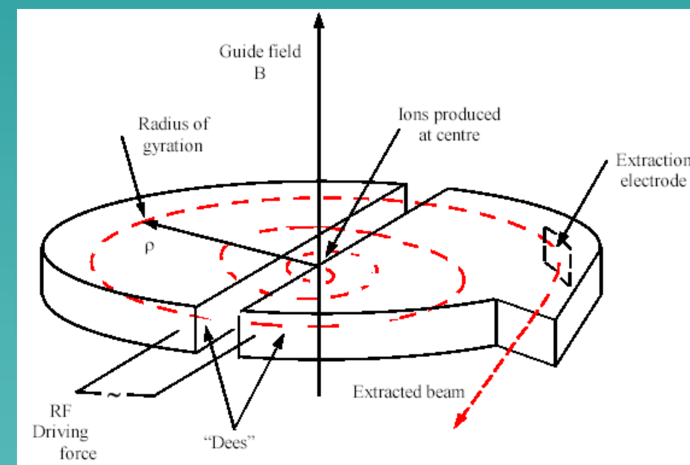


To keep the radius constant during acceleration, the strength of the magnetic field B has to increase synchronously with the beam energy E, $B \propto E$. Therefore, this type of accelerator is called a **synchrotron**.

Cyclotron (The earliest accelerators) 迴旋加速器

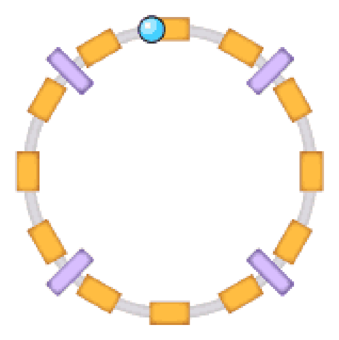
Cyclotron consists of two D-shaped objects (dees) with a potential difference between them. A stream of particles moved in a plane perpendicular to a uniform magnetic field, which bent the particle tracks so that they passed through an electric field in a gap between dees and were accelerated.



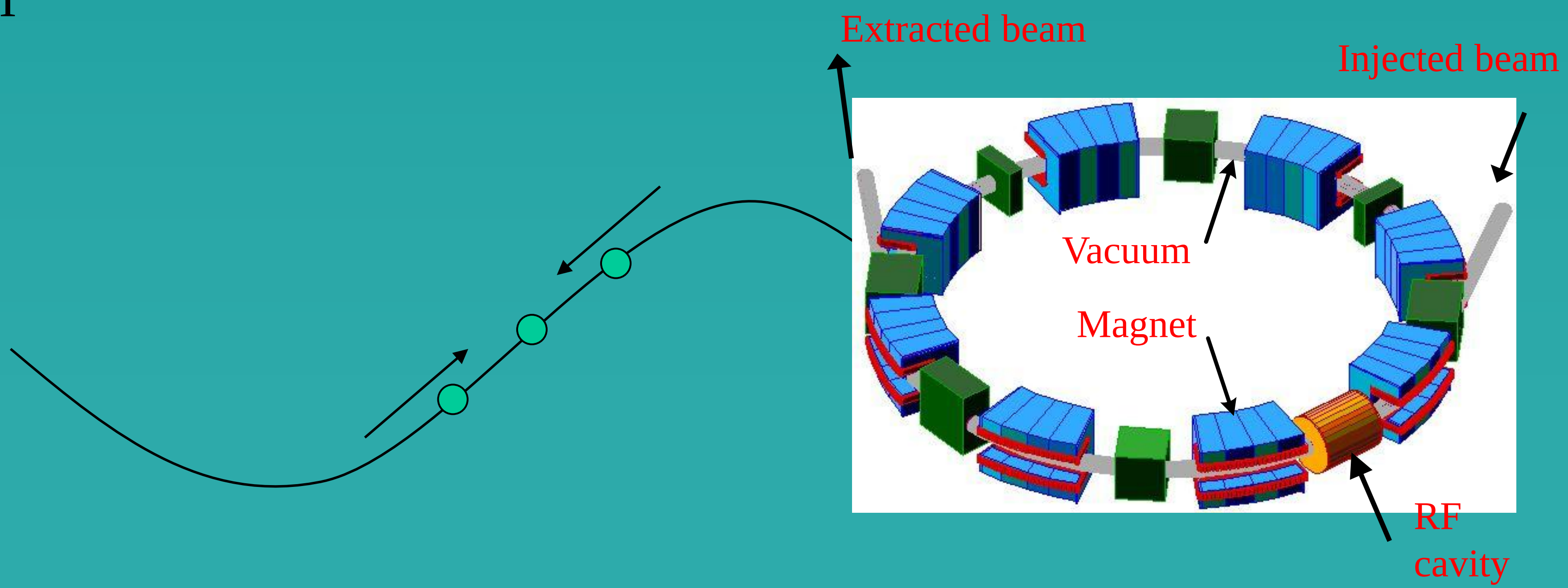


For non-relativistic particles the frequency of the machine was determined by the Lorentz force law, $F = e\,v\,B$, and the formula for centripetal acceleration, $v^2 / r = F / m = e\,v\,B / m$, so the angular frequency is given by: $\omega = e\,B / m$.

Synchrotron 同步加速器

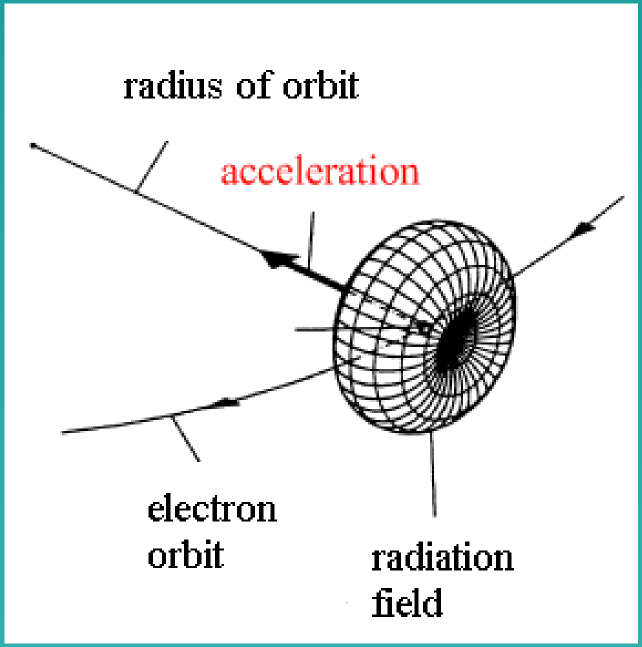


- Particles “ride” an RF wave
  - Slower particles get pushed
  - Faster get slowed
  - Leads to synchrotron oscillations
    - However, “bunches” are formed
  - Transverse instabilities lead to “betatron” oscillations
- Magnets are used to steer the beams during acceleration and during “fill”

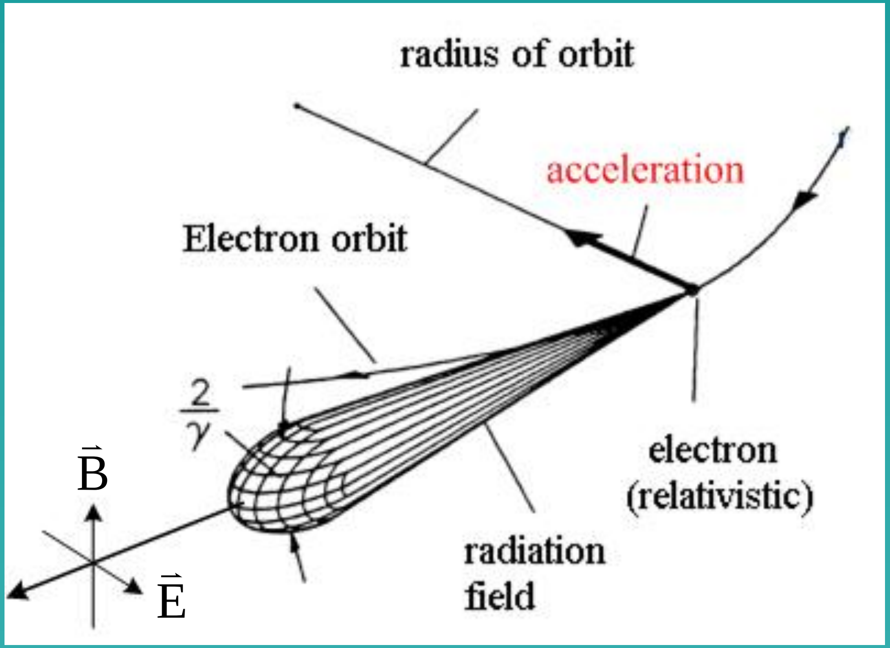


Radiation Fundamental

- When electrons are accelerated (*e.g*. linear acceleration in a radio transmitter antenna) they emit electromagnetic radiation (*i.e*., radio waves) in a rather non-directional pattern
- Electrons in circular motion are also undergoing acceleration (centripetal)



At low electron velocity (non-relativistic case) the radiation is emitted in a non-directional pattern



When the electron velocity approaches the velocity of light, the emission pattern is folded sharply forward. Also the radiated power goes up dramatically

Fields of a Accelerated Charge

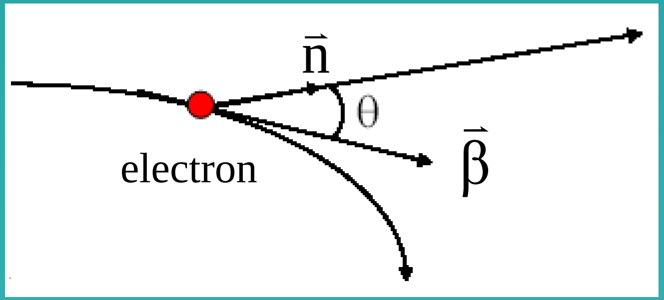
$$\vec{E}(\vec{r},t) = \frac{q}{4\pi\varepsilon_0}\left[\frac{\vec{n}-\vec{\beta}}{(1-\vec{n}\cdot\vec{\beta})^3\gamma^2}\cdot\frac{1}{r^2}\right]$$

Coulomb field

$$+\frac{q}{4\pi\varepsilon_0 c}\left\{\frac{\vec{n}\times[(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}]}{(1-\vec{n}\cdot\vec{\beta})^3\gamma^2}\cdot\frac{1}{r}\right\}$$

Radiation field

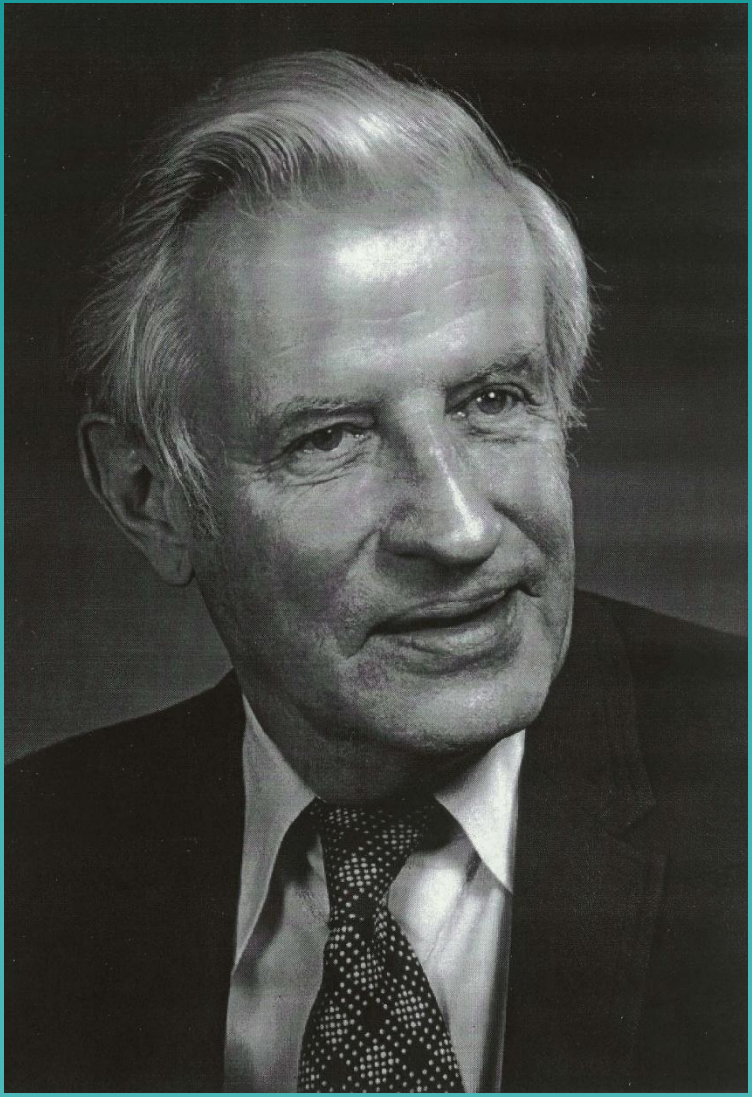
$$\vec{B}(\vec{r},t) = \frac{1}{c}[\vec{n}\times\vec{E}(\vec{r},t)]$$



$$\gamma = \frac{1}{\sqrt{1-\beta^2}}$$

$$\vec{n} = \frac{\vec{r}}{r} \quad , \quad \vec{\beta} = \frac{\vec{v}}{c}$$

John Blewett Observed Effects of Synchrotron Radiation in General Electric 100 MeV Betatron - 1945



PHYSICAL REVIEW VOLUME 69, NUMBERS 3 AND 4 FEBRUARY 1 AND 15, 1946

Radiation Losses in the Induction Electron Accelerator

JOHN P. BLEWETT
Research Laboratory, General Electric Company, Schenectady, New York
(Received September 13, 1945)

This paper discusses the possibility that radiation losses because of the high radial accelerations experienced by the electrons in an induction electron accelerator may introduce limitations in the design of accelerators for energies above 100 million electron volts. The effects of radiation losses on the electron orbits are calculated, and it is shown that not only should the orbit shift pulse necessary to bring electrons to a target inside the equilibrium orbit fall below the value expected in the absence of radiation, but also electrons should eventually arrive at the target with no orbit shift pulse whatever, at a phase of the field wave predictable from the theory. Both effects have been observed in the General Electric 100-Mev unit in a manner consistent with the predictions of the theory. The radiation itself has not yet been detected.

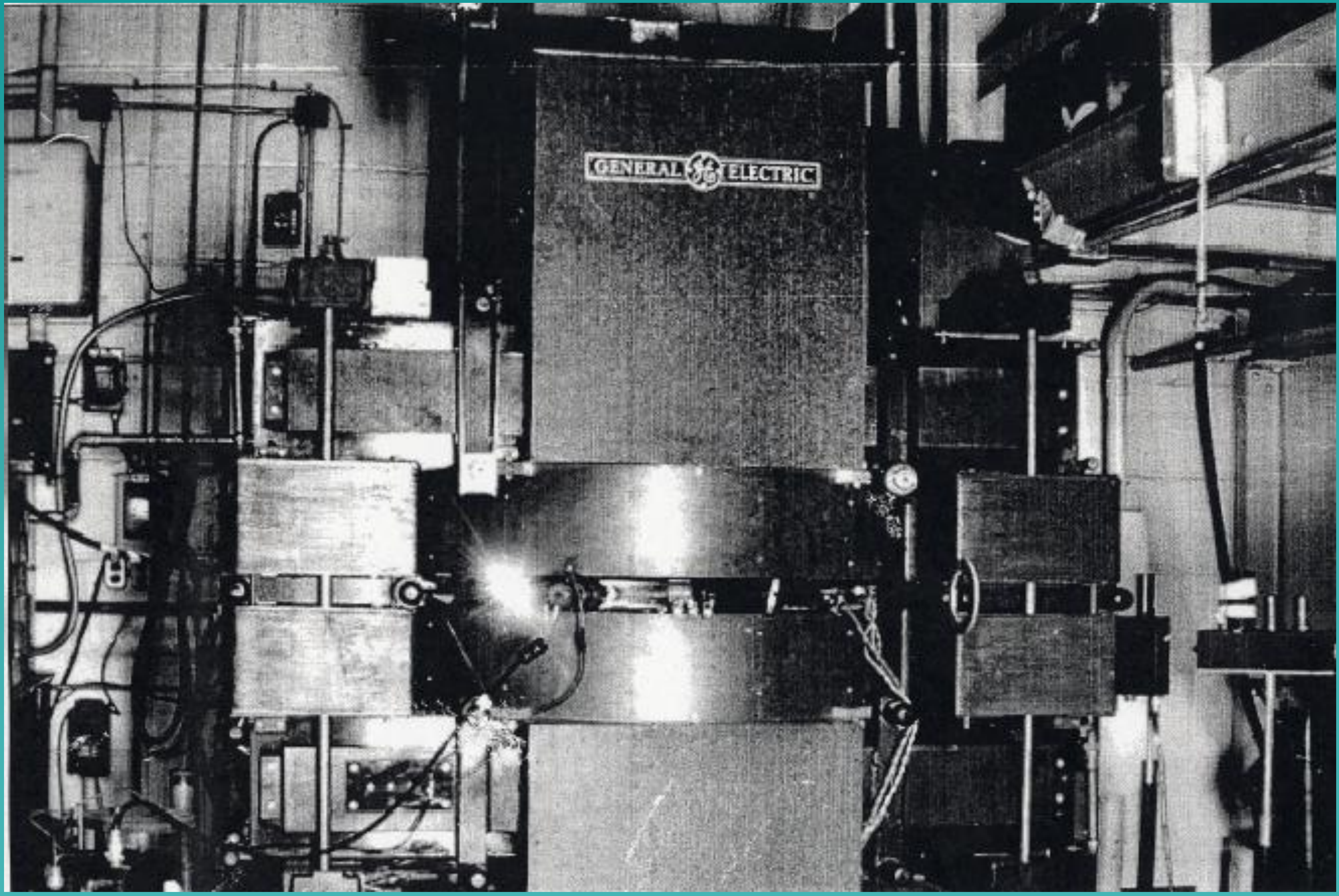
1. INTRODUCTION*

IN the induction electron accelerator, the electrons are subjected continually to radial accelerations of the order of 10^{17} meters per second per second. It has been pointed out by

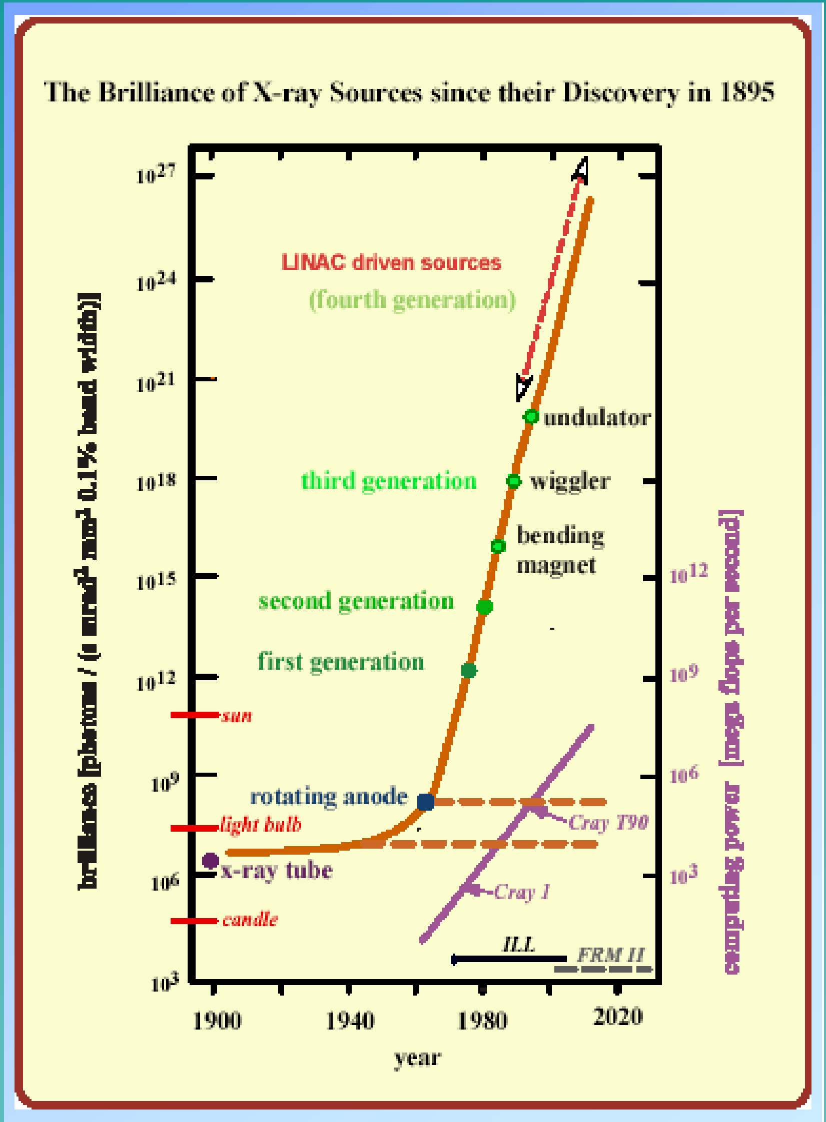
* *Symbols:*—Unrationalized m.k.s. units will be used throughout: The following symbols will be employed:

A = peak value of applied magnetic flux density at the equilibrium orbit (webers per sq. m)
A' = peak value of magnetic flux in orbit shrinking pulse at the equilibrium orbit (webers per sq. m)
B_0 = applied magnetic flux density at the equilibrium orbit (webers per sq. m)
B_r and B_z are components of magnetic flux density (webers per sq. m)
c = velocity of light = 3.00×10^8 m per sec.
e = charge on the electron = 1.602×10^{-19} Coulomb
E_r and E_z are components of electric field (volts per m)
f_n and f_t are normal and tangential components of the acceleration vector $\mathbf{f}$ (m per sec. per sec.)
$F(\omega t) = (\omega t/\sin\omega t) - \cos\omega t - (2/3)\sin^2\omega t\cos\omega t$
h = Planck's constant = 6.624×10^{-34} joule sec.
H_r and H_z are components of magnetic field
I = beam current (amperes)
m_0 = rest mass of the electron = 9.107×10^{-31} kg

Synchrotron Radiation was first observed in 1947 by Elder, Gurewitsch, Langmuir and Pollock in a 70MeV synchrotron.



History of Synchrotron Radiation



Zeroth generation sources

1950's-60's: Electron synchrotrons (cyclic accelerators)

First generation sources (storage rings)

1970's: e+/e- colliders (Mostly parasitic on high energy physics programs)

Second generation sources

1980's: New rings and fully dedicated use of e+/e- colliders, use of wigglers & undulators

Third generation sources

1990's: Low emittance ring with many straight sections for insertion devices

Fourth generation sources

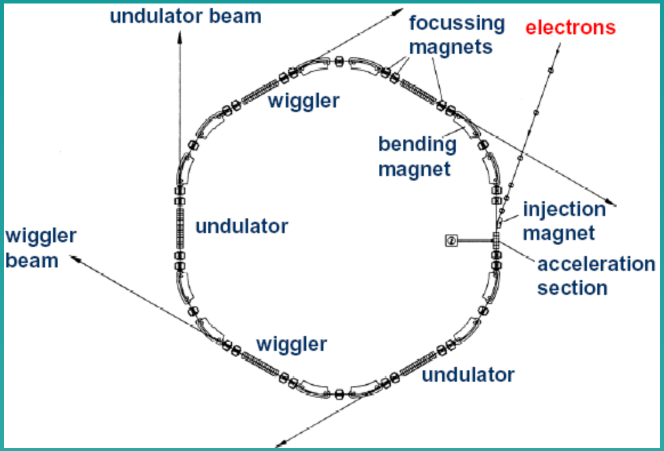
2000's: Linac-based sources

- Free-electron laser (FEL)
- Energy Recovery Linac (ERL)

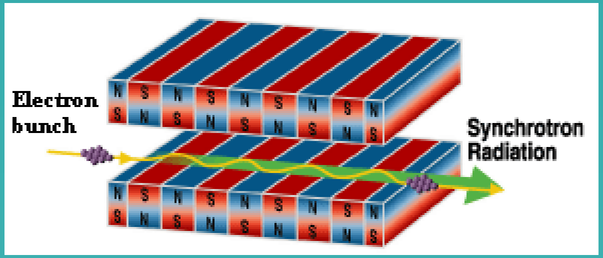
Diffraction-limited rings; Ultra-short bunches; New ideas

Bending magnet(偏轉磁鐵) & insertion device(插件)

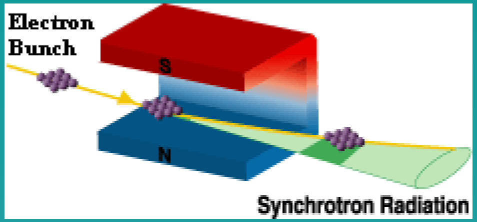
Storing Ring



Undulator / Wiggler



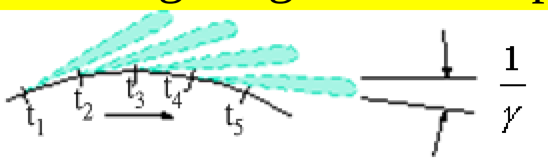
- Bending Magnet
  - White X-rays
  - Wide horizontal divergence
  - 1/γ limited vertical divergence
  - Moderate power
  - Moderate power density



- Wiggler
  - White X-rays
  - Moderate horizontal divergence
  - 1/γ Limited vertical divergence
  - High power
  - High power density
  - Elliptically polarized/linearly polarized
- Undulator
  - Quasi-monochromatic X-rays
  - Small vertical and horizontal divergence (Central Cone)
  - High power
  - Extremely high power density
  - Circularly polarized/ linearly polarized

Three forms of Synchrotron Radiation

Bending Magnet: a sweeping searchlight

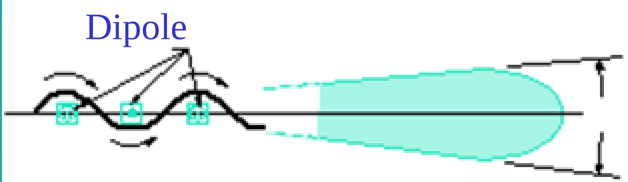


Continuous spectrum

Critical energy $E_c = \hbar\omega_c = \dfrac{3e\hbar B\gamma^2}{2m}$

$E_c(\text{keV}) = 0.665\, B(\text{T}) E^2(\text{GeV})$

Wiggler: incoherent superposition



$>> \dfrac{1}{\gamma}$

eg: for B = 1.35T, E = 2GeV

E_c = 3.6keV

增頻磁鐵

B increases ➔ E_c increases

Undulator: coherent superpositiom

$\dfrac{1}{\gamma\sqrt{N}}$

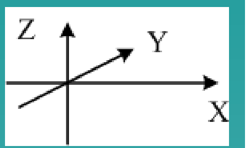
Quasi-monochromatic spectrum with peaks at lower energy than a wiggler

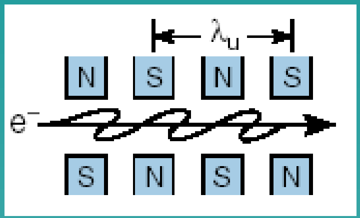
聚頻磁鐵

$$\lambda = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right)$$

Undulator radiation

Laboratory
Frame of Reference



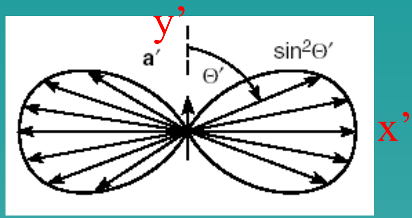


Lorentz transformation

$$E = \gamma mc^2$$

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

Frame
of Moving Electron

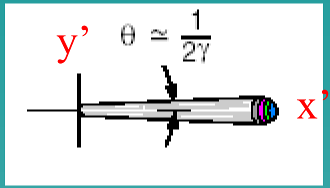


Electron radiates at the Lorentzed contrated wavelength

$$\lambda' = \frac{\lambda_u}{\gamma}$$

Bandwidth $\frac{\lambda'}{\Delta\lambda'} \cong N$

Laboratory
Frame of Reference



Doppler shortened Wavelength on axis

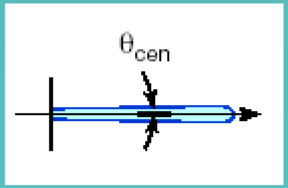
$$\lambda = \lambda'\gamma(1-\beta\cos\theta) = \frac{\lambda_\mu}{2\gamma^2}(1+\gamma^2\theta^2)$$

Accounting for transverse Motion due to the periodic Magnetic field

$$\lambda = \frac{\lambda_u}{2\gamma^2}(1+\frac{K^2}{2}+\gamma^2\theta^2)$$

$$K = \frac{eB_0\lambda_u}{2\pi mc}$$

Following
Monochromator



$$\theta_{cen} \cong \frac{1}{\gamma\sqrt{N}}$$

Synchrotron radiation - basic properties

1.High flux and brightness

2.High stability

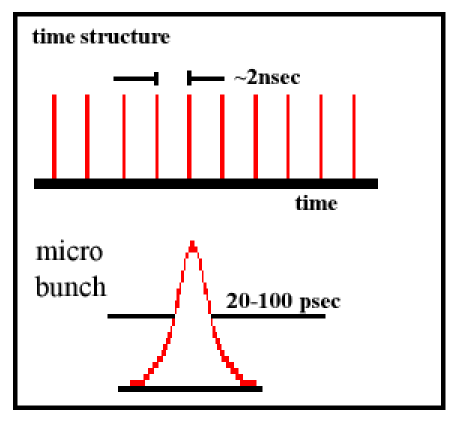
3.Broad spectral range

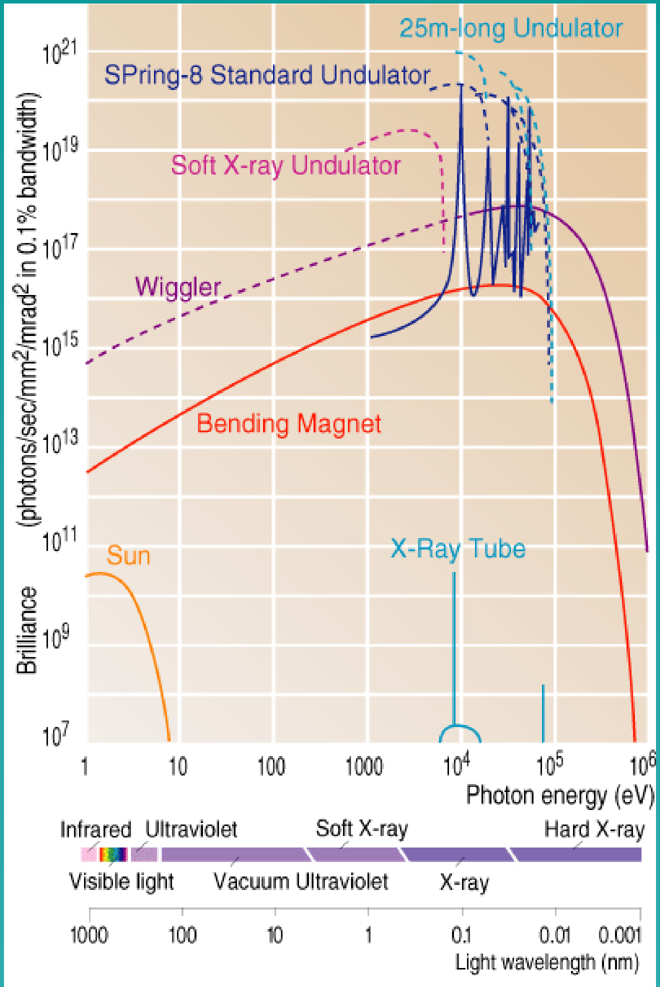
4.Small source size

5.Partial coherence

6.Polarized (linear, elliptical, circular)

7.Pulsed time structure





Flux = $\dfrac{\text{\# of photons in given } \Delta\lambda/\lambda}{\text{sec, mrad } \theta}$

Brightness = $\dfrac{\text{\# of photons in given } \Delta\lambda/\lambda}{\text{sec, mrad } \theta\text{, mrad } \varphi\text{, mm}^2}$

Temporal and Spatial coherence 同調性

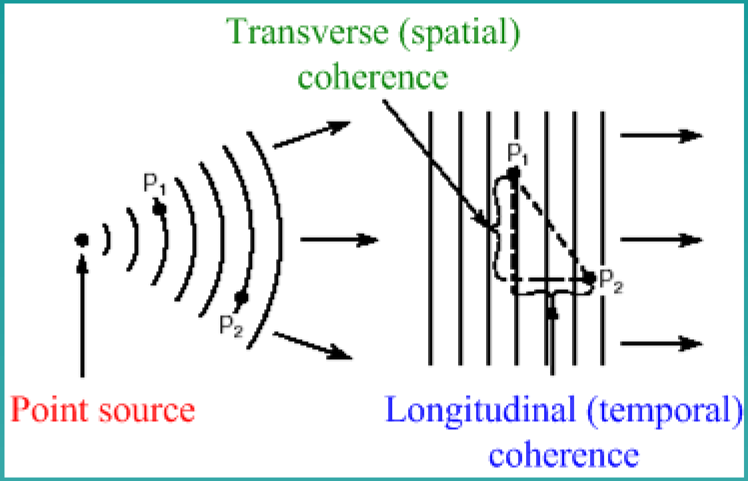
Mutual coherence factor

$$\Gamma_{12}(\tau) \equiv < E_1(t) E_2^*(t+\tau) >$$

Normalized degree of spatial coherence

$$\gamma_{12}(\tau) = \frac{< E_1(t) E_2^*(t+\tau) >}{\sqrt{<| E_1(t) |^2>} \cdot \sqrt{<| E_2(t) |^2>}}$$

Incoherent	$\gamma_{12} = 0$
Partially coherent	$\gamma_{12} < 1$
Fully coherent	$\gamma_{12} = 1$



Longitudinal coherence length

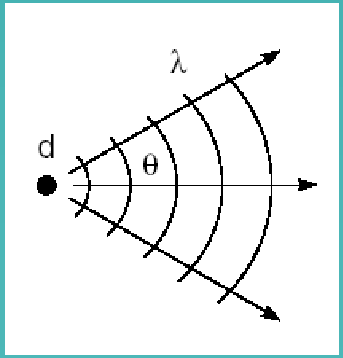
$$l_{coh} = \frac{\lambda^2}{2\Delta\lambda}$$

Transverse coherence length (θ)

$$d \cdot \theta = \frac{\lambda}{2\pi}$$

(The uncertainty principle)

d: source size



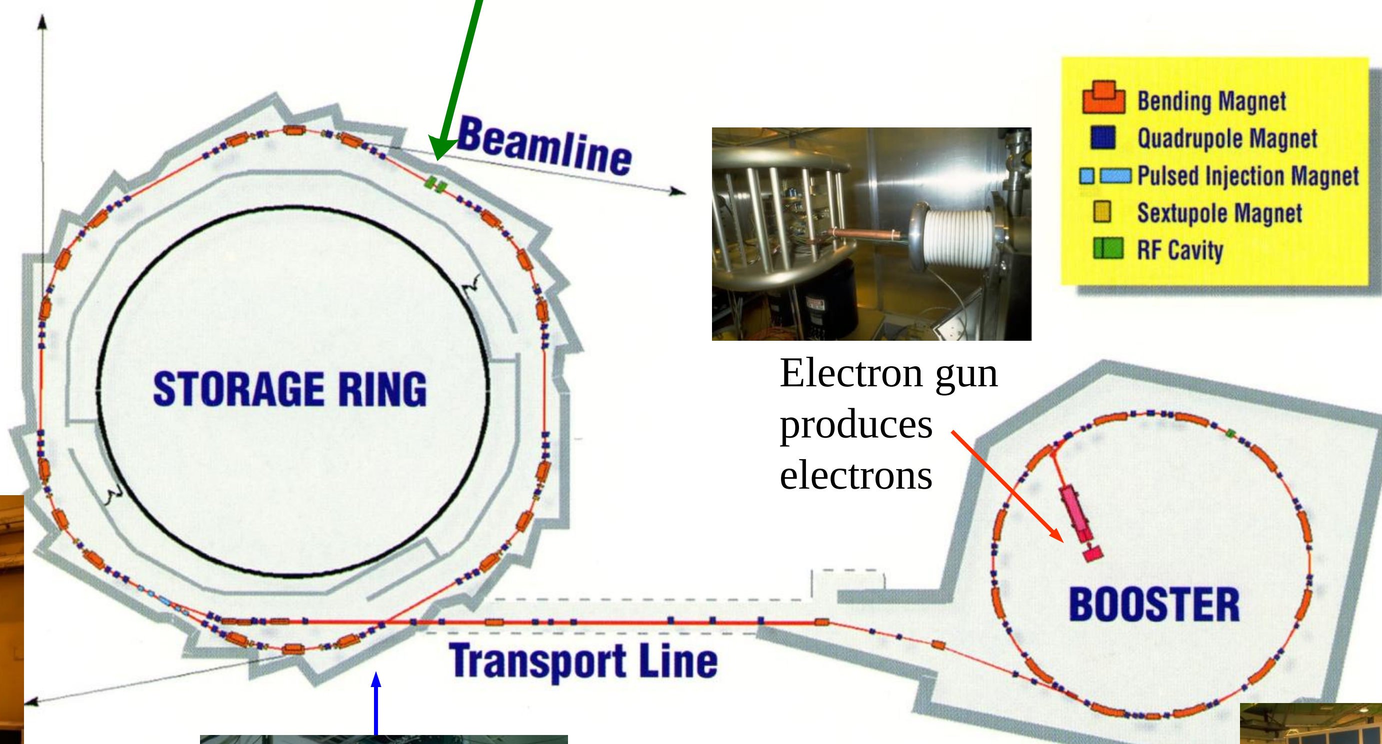
NSRRC

1.5 GeV; $\gamma = 3000$; 120 m circumference

How is it Practically Produced and Used for Research?

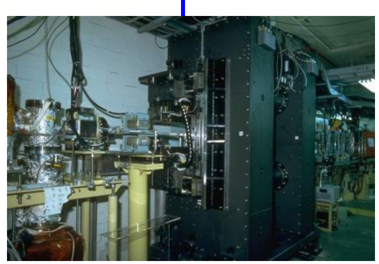
The storage ring circulates electrons, where they are bent, synchrotron radiation is produced

Klystrons generate high power radio wave to sustain electron acceleration, replenishing energy lost to synchrotron radiation



Electron gun produces electrons

Beam lines transport radiation into “hutches”, where instrumentation is available for experiments

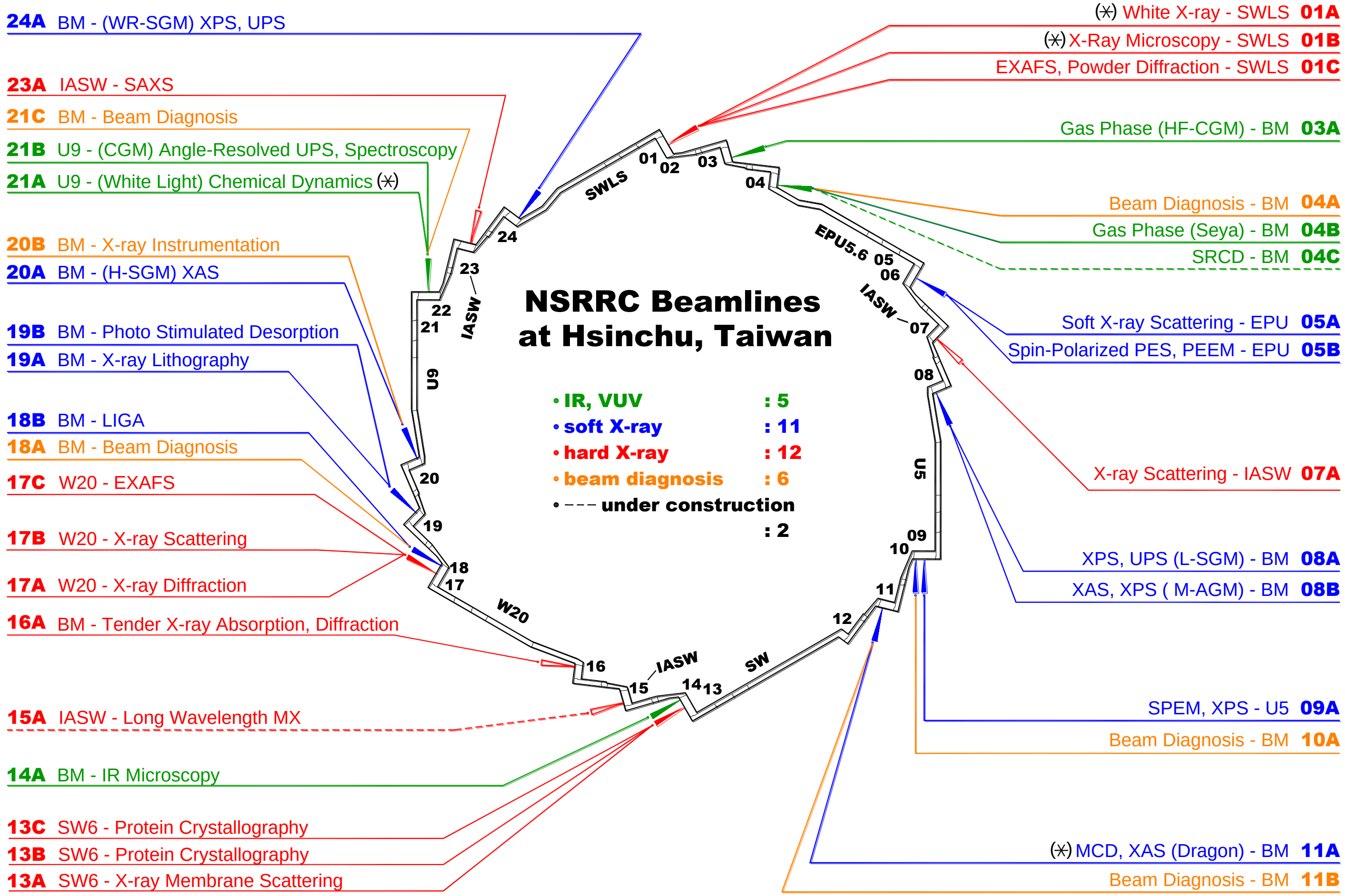


Wiggler / Undulator insertion devices generate strong x-ray beams

Linear accelerator/ booster accelerate e^- which are transported to storage ring

NSRRC TLS Beamlines Layout

30 BLs, over 50 End stations



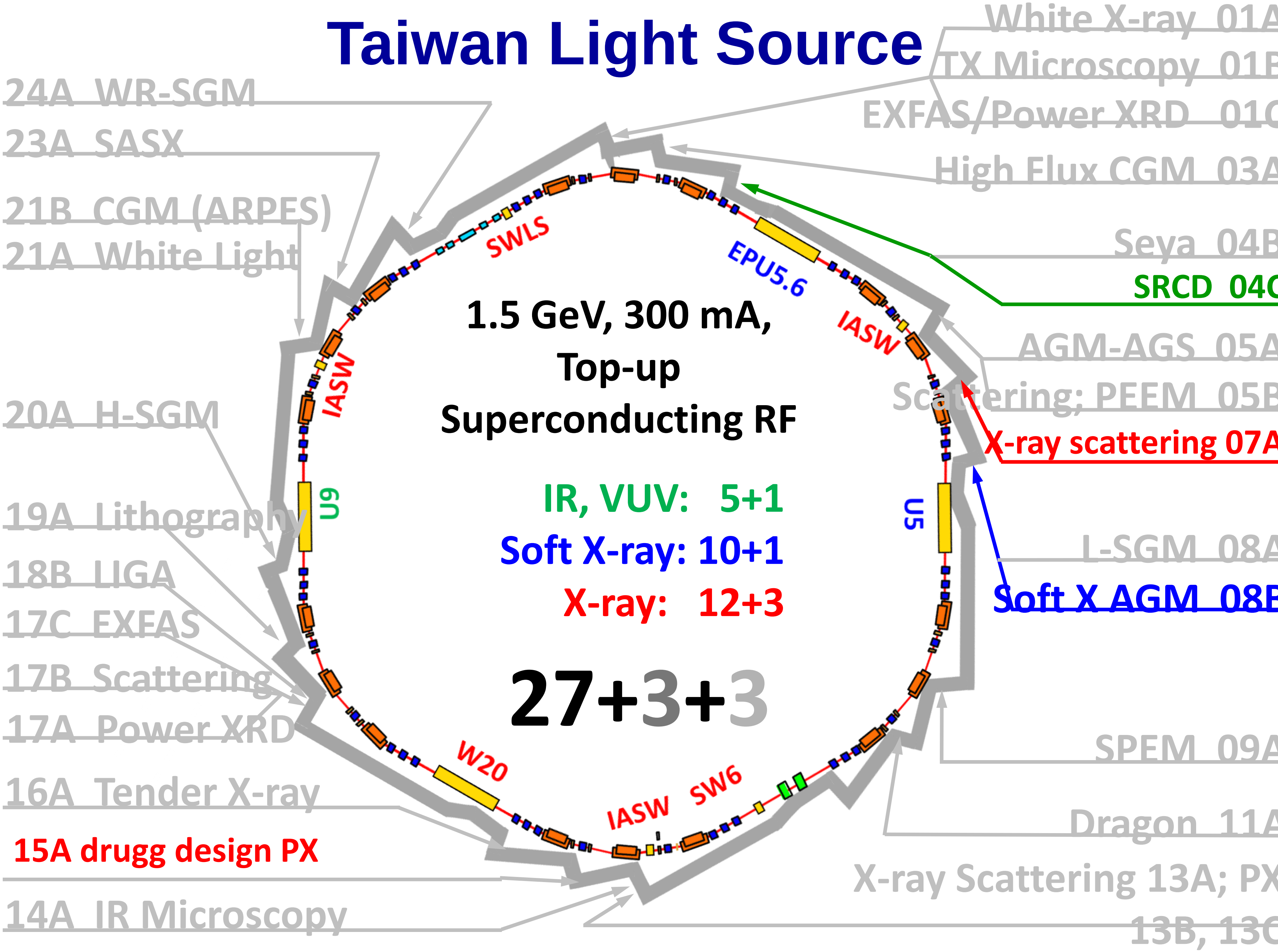
3 additional hard x-ray BLs at SPring-8, Japan

Insertion Devices

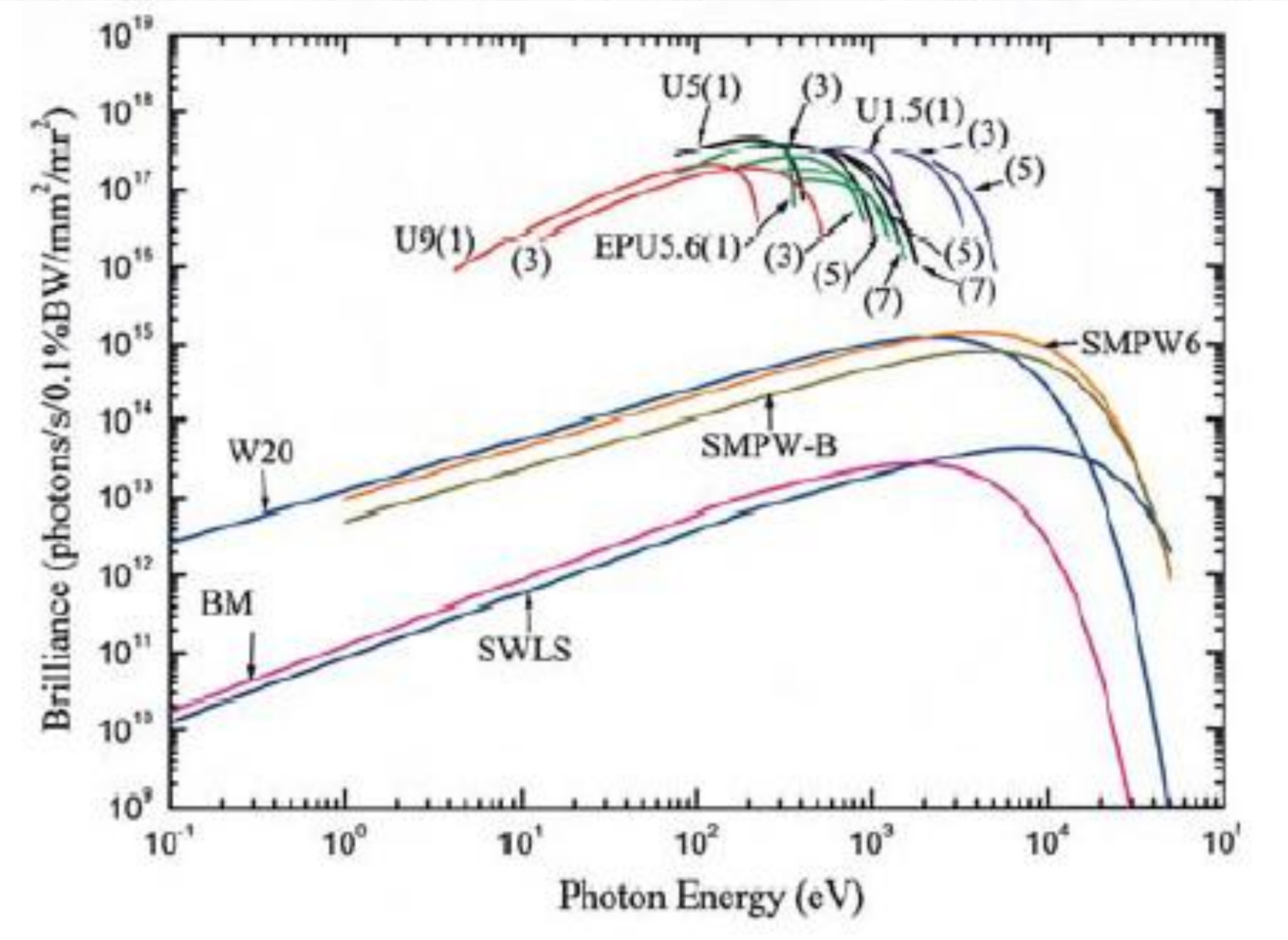
EPU5.6: Elliptically Polarized Undulator
IASW: In-Archomatic Superconducting Wiggler
SW: Superconducting Wiggler (3.2 T, 32 Poles)
SWLS: Superconducting Wavelength Shifter
U5: Undulator (5 cm, 76 Periods)
U9: Undulator (9 cm, 48 Periods)
W20: Wiggler (1.8 T, 27 Poles)

(*) : Participating Research Group

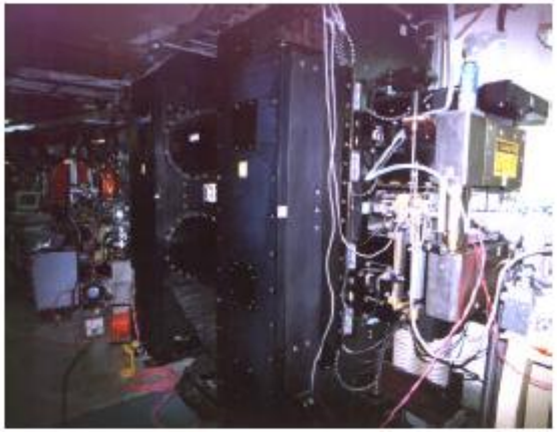
Taiwan Light Source



NSRRC Photon Spectrum from Insertion Devices



NSRRC Insertion Devices



W20 wiggler

U10 undulator

U5 undulator

U9 undulator

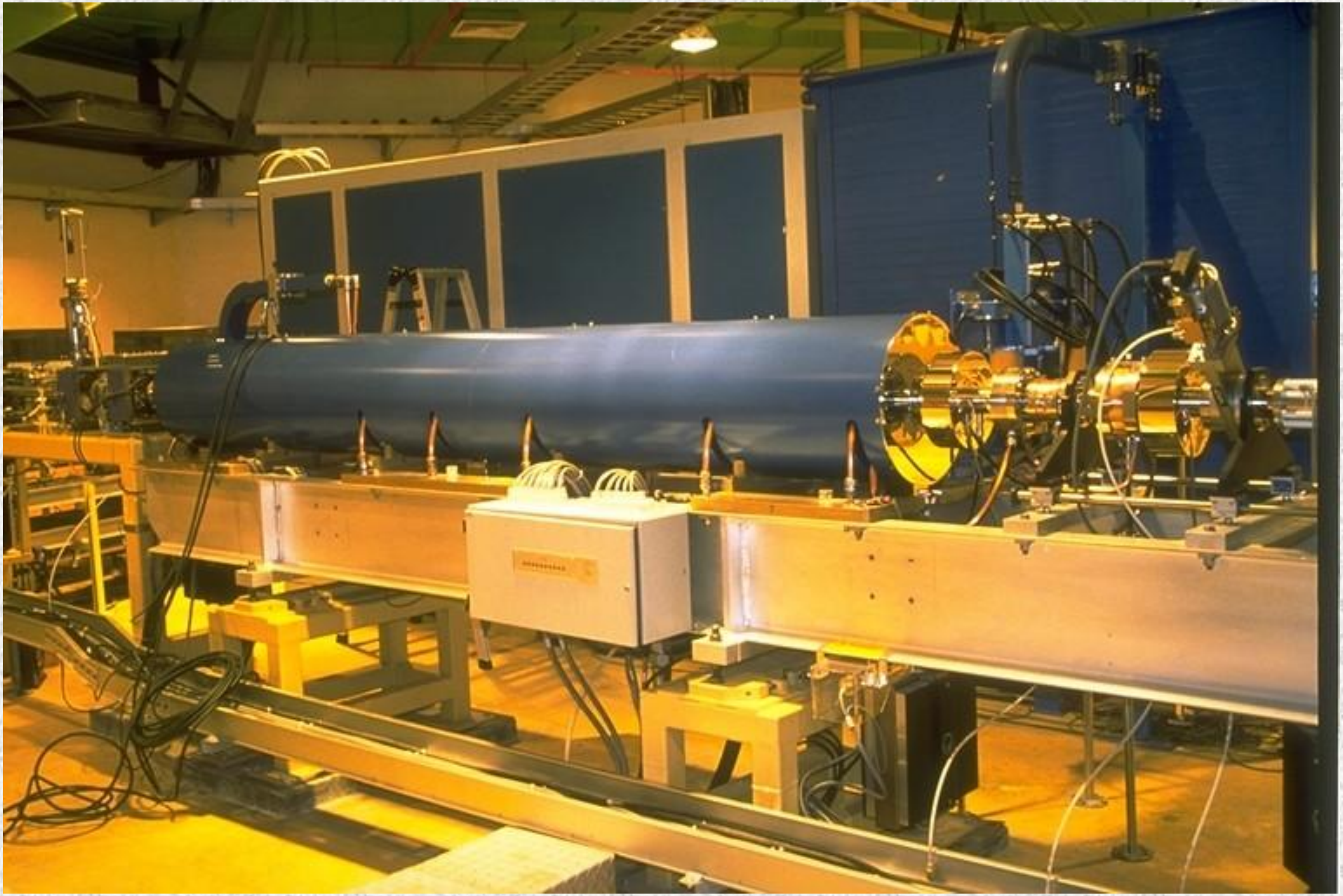
EPU5.6 undulator

IVXU3.2 undulator

Parameters of the Insertion Devices

	W20	U10	U5	U9	EPU5.6	SWLS	SW6
Type	Hybrid	Hybrid	Hybrid	Hybrid	Pure	SC	SC
λ [cm]	20	10	5	9	5.6	32.56	6
Gap [mm]	22	22	18	18	18	56	18
N	13	20	76	48	66	1.5	32
Photon energy (keV)	4-15	----	0.06-1.5	0.004-0.5	0.06-1.5	4-33	6.5-19
Deflection K	33.6	9.34	2.99	10.5	3.5 (2.35)	----	17.9
$B_{max.}$ [T]	1.8	1.0	0.64	1.25	0.67 (0.45)	6	3.2
Phase error Θ	N/A	2.5°	3°	3.7°	5.5°	N/A	N/A
$\theta_x(\theta_y)$ [μrad]	N/A	15 (6)	6 (11)	20 (10)	10 (15)	N/A	N/A
δ_x (δ_y) [μm]	N/A	5 (2)	7 (10)	8 (2)	2 (1)	N/A	N/A
Beam duct aperture(mm^2)	17x80	17x80	13x80	13x80	13x80	20x100	11x80
Installation	Dec.1994	Oct.1995	Mar.1997	Apr.1999	Sep.1999	Apr. 2002	Jan. 2004

NSRRC Linear Accelerator

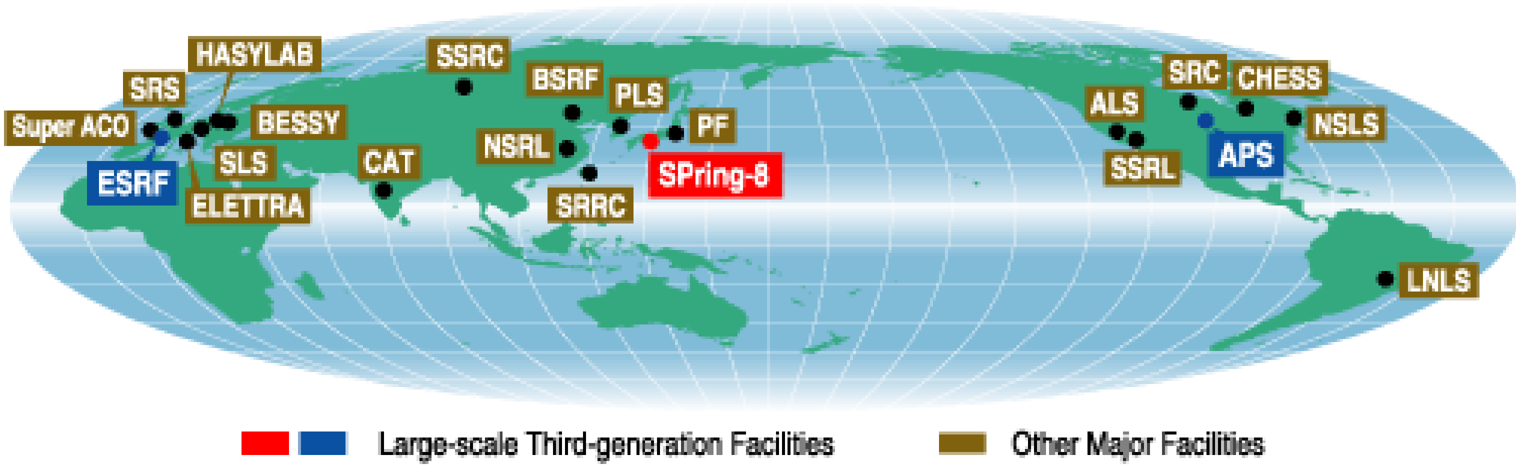


50 Mev

NSRRC Booster Synchrotron

Focusing Magnet

Synchrotron Radiation Centres around the world



SR sources around the world

http://www.spring8.or.jp/ENGLISH/general_info/overview/sr.html

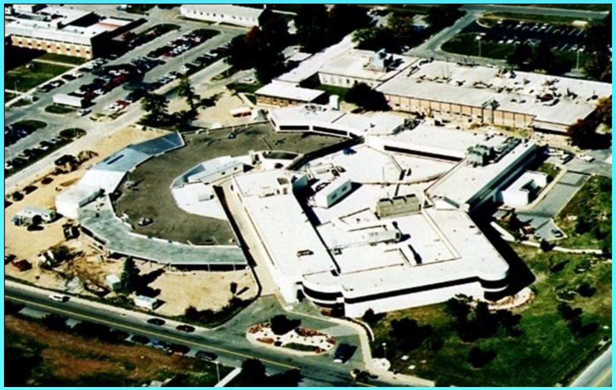
Synchrotron Radiation Centers in USA

1.9 GeV, γ = 3720, 197 m circumference

Advanced Light Source (ALS),
Lawrence Berkeley National Laboratory (1993)

Two US 3rd Generation facilities - among the world's first

Advanced Photon Source (APS),
Argonne National Laboratory (1996)



National Synchrotron Light Source (NSLS),
Brookhaven National Laboratory (1982)

First US 2nd Generation facility

Stanford Synchrotron Radiation Laboratory (SSRL),
Stanford Linear Accelerator Center (1974)

World's first SR storage ring x-ray user facility

European Synchrotron Radiation Facility (ESRF)

6 GeV; γ = 11800; 884m circumference

Spring-8 (Super Photon ring-8 GeV) Japan

8 GeV; γ = 15,700; 1.44 km circumference

X光繞射
X-ray Diffraction

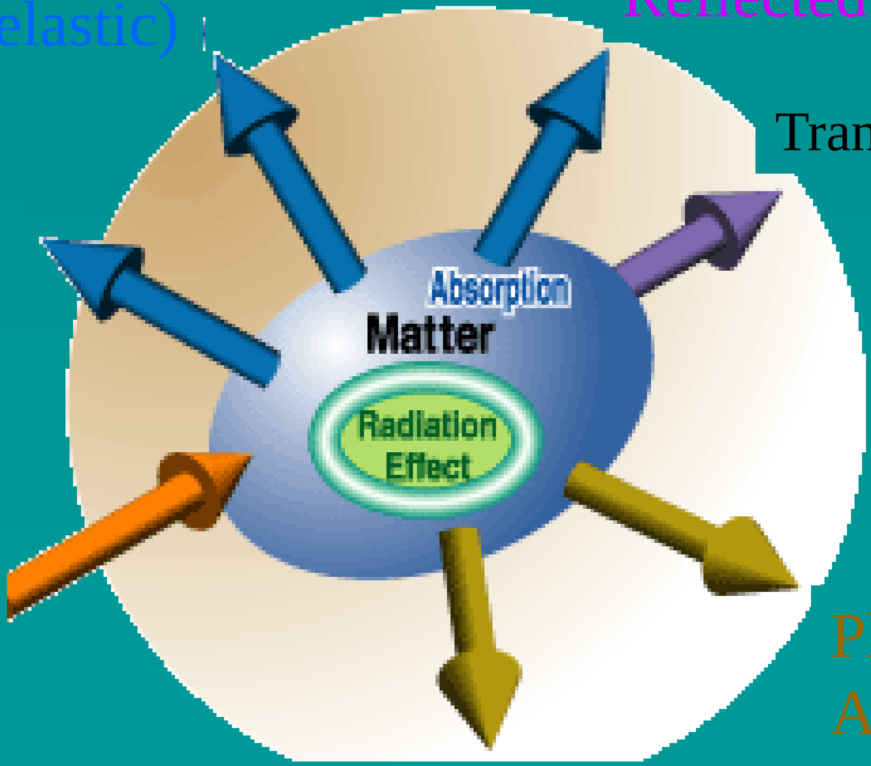
Interaction between x-rays and matter

Scattered x-rays
(elastic / inelastic)

Reflected x-rays

Transmitted / Refracted X-rays

Diffracted X-rays



Incident x-rays

光電子
Photoelectron emission
Auger electron emission

Fluorescence
螢光

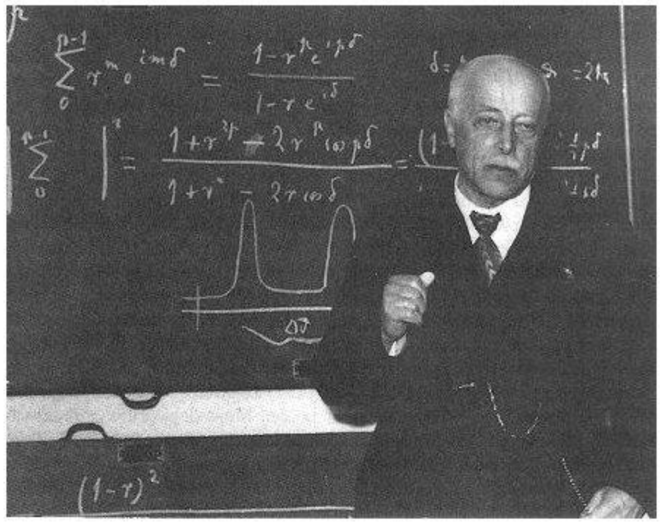
Discovery of X-ray Diffraction

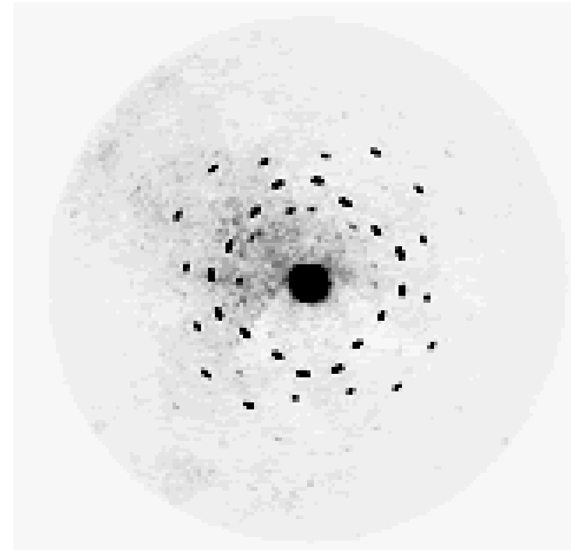
The Nobel Prize in physics 1914

"for his discovery of the diffraction of x-rays by crystals"

Max Von Laue

(1879-1960)
Germany





Interference pattern observed by von Laue and collaborators using a photographic plate in 1912. The large central spot is due to the unscattered X-ray beam. The dark spots correspond to directions where x-rays scattered from crystal (ZnS) layers interfere constructively.

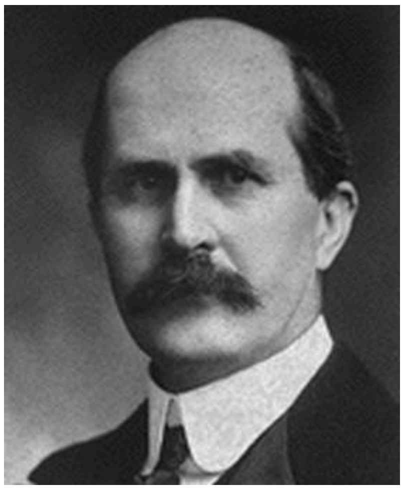
http://www.nobel.se/physics/educational/x-rays/what-4.html

Analysis of Crystal Structure

The Nobel Prize in physics 1915

"for their service in analysis of crystal structure by means of x-rays"

Sir William Henry Bragg



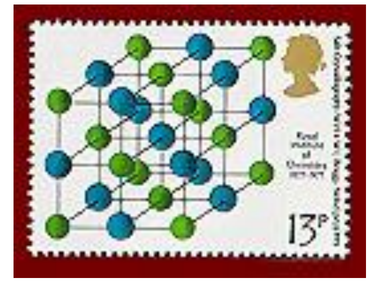
(1862-1942)

United Kingdom

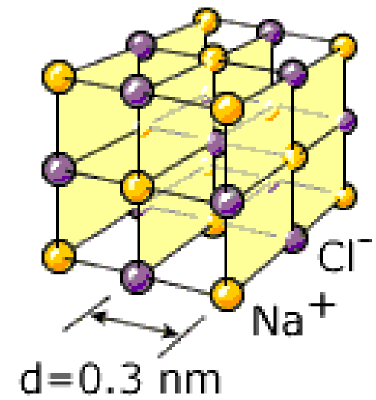
Sir William Lawrence Bragg

(1890-1971)

United Kingdom



NaCl



Determining the crystal structure NaCl, ZnS, Diamond,…

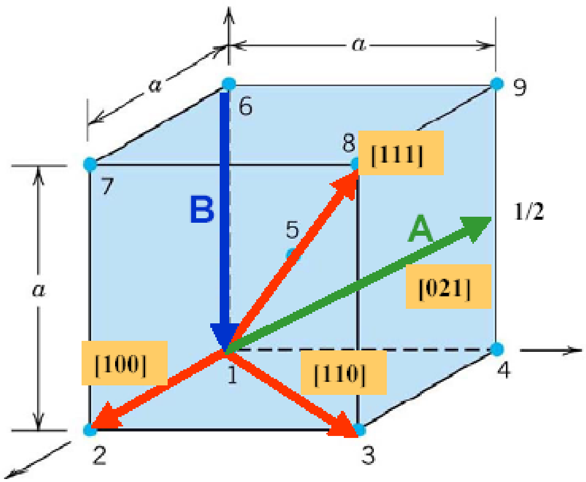
http://www.nobel.se/physics/laureates/1915/

http://www.nobel.se/physics/educational/x-rays/what-6.html

Crystal Systems- Body-Centered Cubic (BCC)

- Indexing crystallographic directions

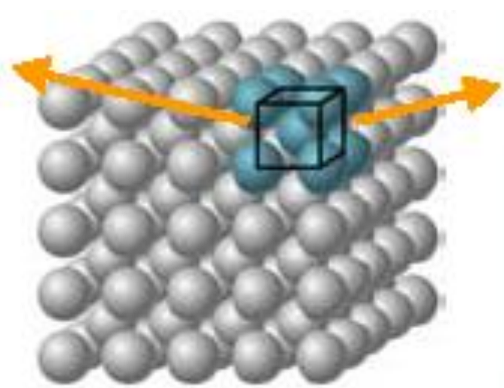
Miller indices

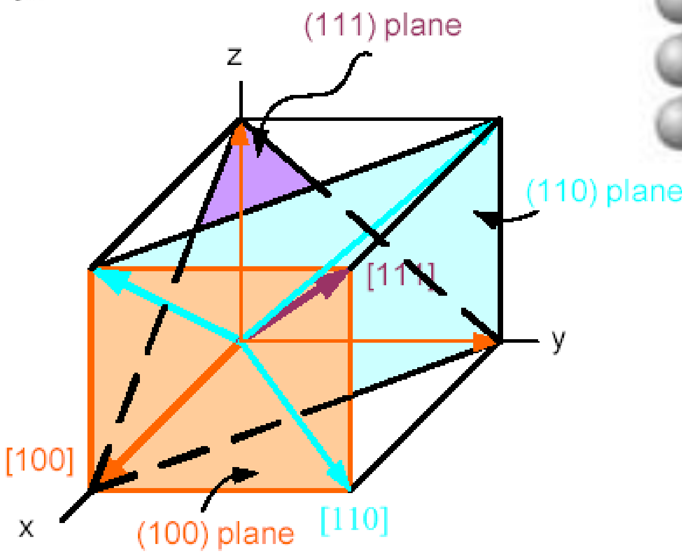


direction A = [021]

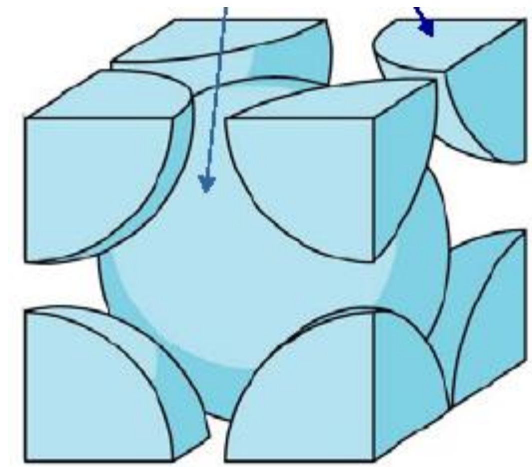
direction B = $[00\bar{1}]$

- Crystal



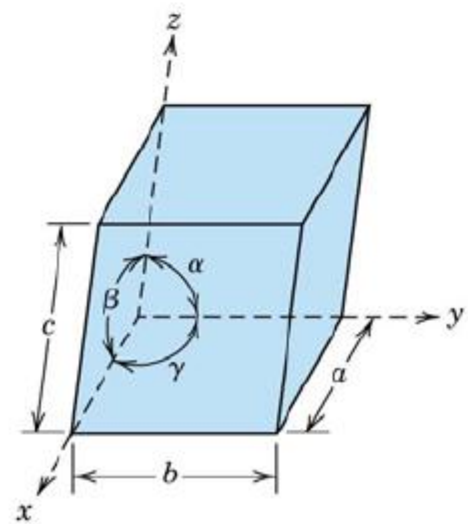


- Unit cell



- Lattice constant

a, b, c, α, β, γ

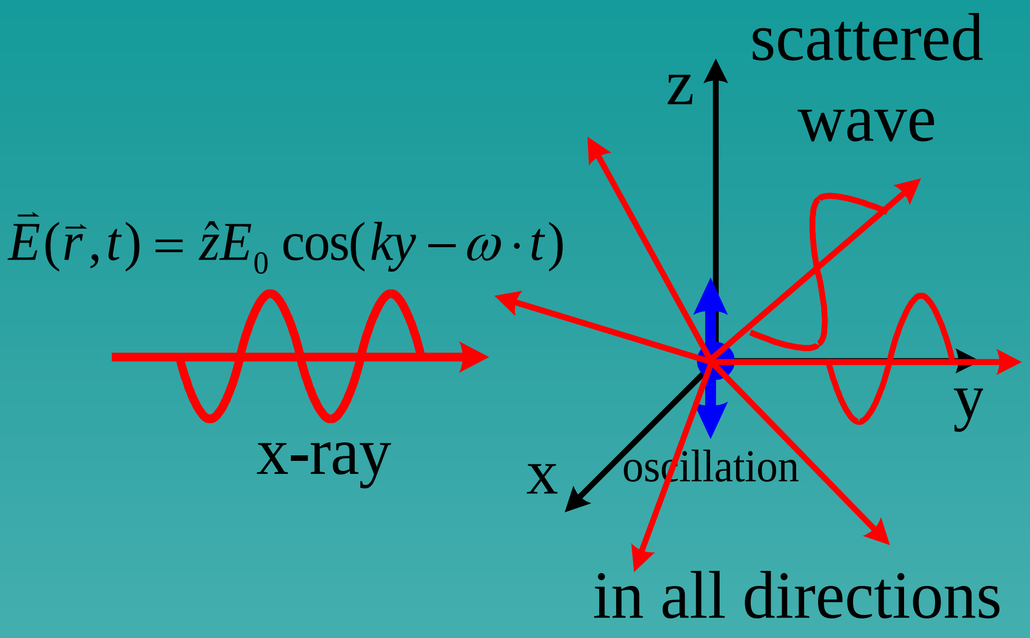


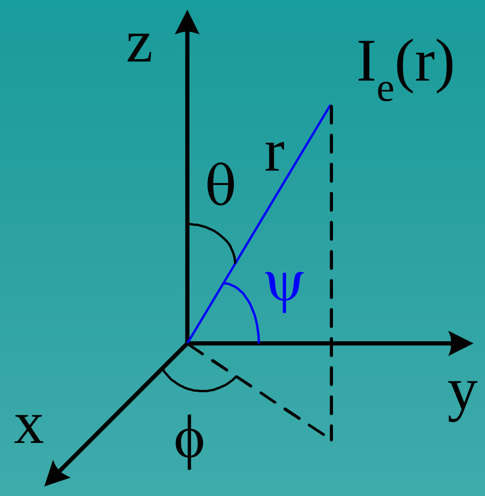
3D: 14 Bravais Lattices, 7 Crystal Systems

Bravais Lattice: an infinite array of discrete points with an arrangement and orientation that appears exactly the same from whichever of the points the array is viewed.

Name	**Number of Bravais lattices**	**Conditions**
Triclinic	1 (P)	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2 (P, C)	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = 90^\circ \neq \gamma$
Orthorhombic	4 (P, F, I, A)	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2 (P, I)	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	3 (P, F, I)	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1 (P)	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$
Hexagonal	1 (P)	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

Scattering from one electron





J. J. Thomson (1906) analyzed scattering in detail. Scattered intensity at a distance, r, from a single electron for an unpolarized source is

$$I_e(r) = I_0 \frac{K}{r^2} \left(\frac{1+\cos^2\psi}{2}\right)$$

$$K = 7.94 \times 10^{-30} m^2$$

Thomson scattering

Electric field of incident beam

$$\vec{E}_i = \hat{e}_0 E_0 e^{i(\vec{k}\cdot\vec{r}-\omega\cdot t)}$$

Radiation field scattered by the electron

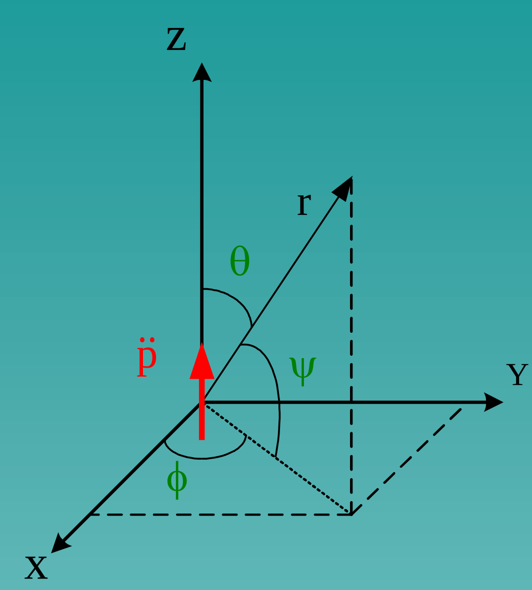
$$\vec{E}(\vec{r},t) = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{c^2 r^3}[\vec{r}\times(\vec{r}\times\ddot{\vec{r}})]$$

$$= -\frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0}{mrc^2}[\hat{n}\times(\hat{n}\times\hat{e}_0)]e^{i(\vec{k}\cdot\vec{r}-\omega\cdot t)}$$

$$= \vec{E}_s(\vec{r},t)e^{i(\vec{k}\cdot\vec{r}-\omega\cdot t)} \quad , \quad \hat{n} = \frac{\vec{r}}{r}$$

$$\vec{B}(\vec{r},t) = \frac{1}{c}\hat{n}\times\vec{E}_s(\vec{r},t)e^{i(\vec{k}\cdot\vec{r}-\omega\cdot t)}$$

$$\vec{E}_s(\vec{r},t) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2}\frac{E_0}{r}[\hat{n}\times(\hat{n}\times\hat{e}_0)]$$



$$m\ddot{\vec{r}} = -e\vec{E}_i$$

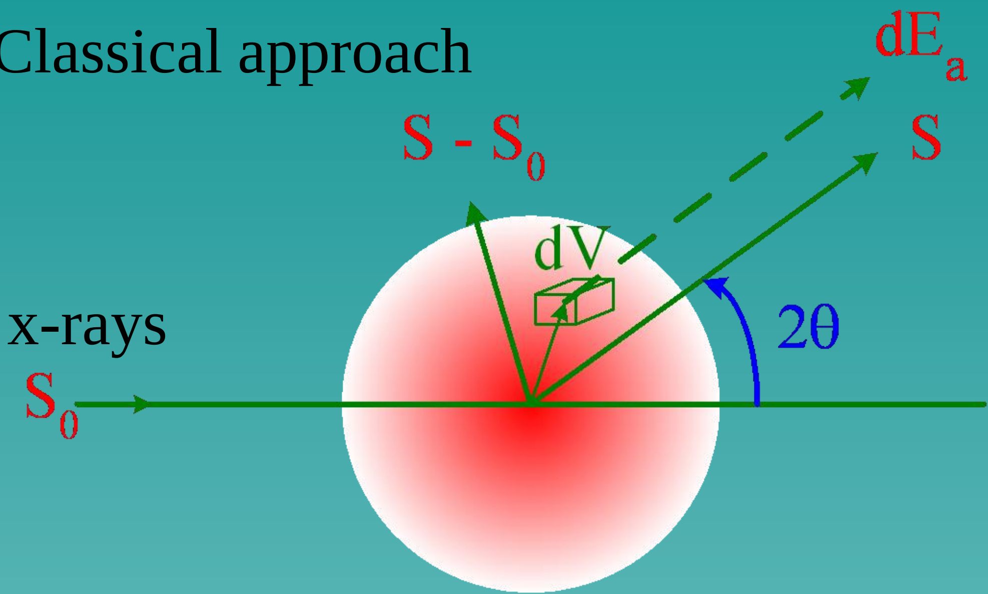
$$\vec{r} = \hat{e}_0 \frac{eE_0}{m\omega^2} e^{-i\omega\cdot t}$$

$$r_c = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2}$$

$$= 2.82\times10^{-15} m$$

Scattering from one atom

Classical approach



ρ(r): charge density of an atom

Assuming ρ(r) is spherically symmetric

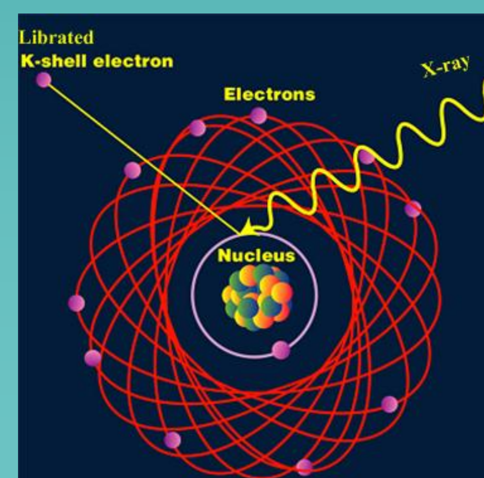
E$_a$(s): Scattering amplitude from one atom

E$_e$(s): Scattering amplitude from one electron

$$E_a(S) = E_e(S) \int_{atom} \rho(r) e^{i\vec{S}\cdot\vec{r}} dV$$

$$= E_e(S) \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \rho(r) r^2 e^{i2\pi rs\cos\theta} \sin\theta dr d\theta d\phi$$

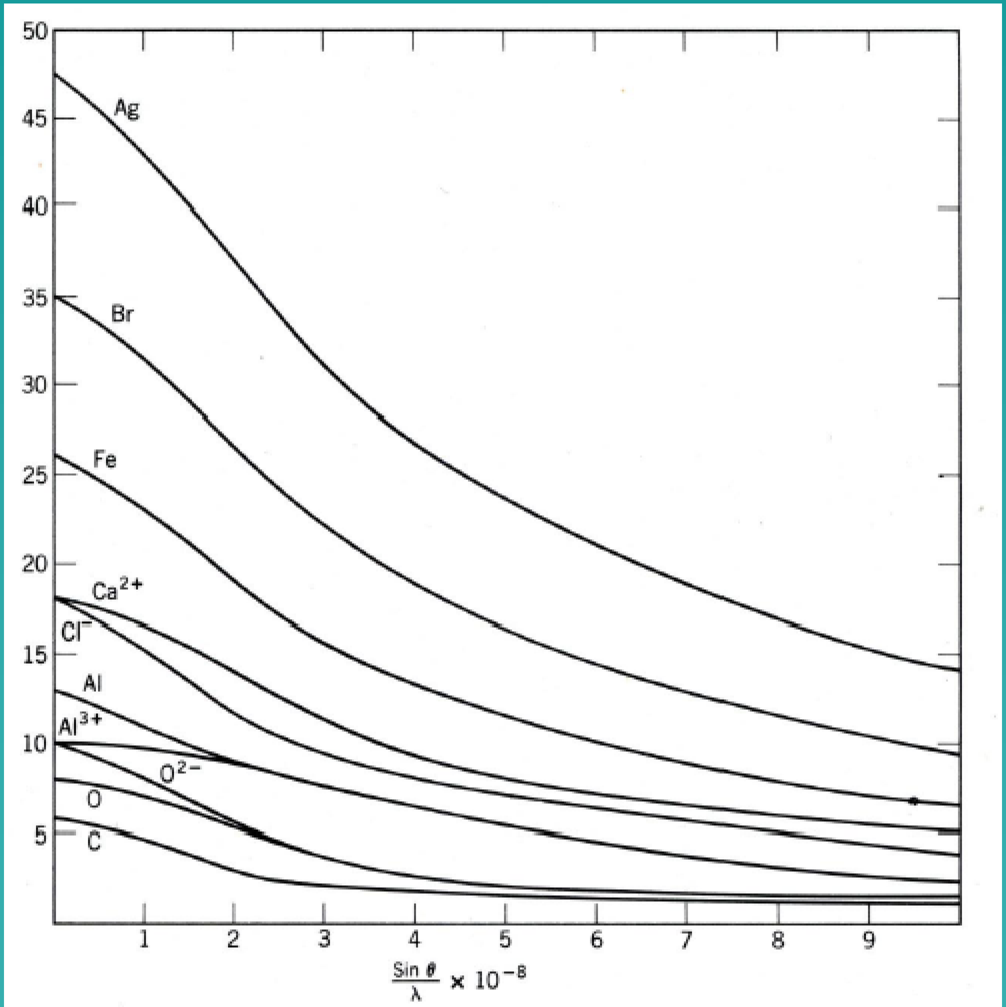
$$= 4\pi \cdot E_e(S) \int_{r=0}^{\infty} \rho(r) r^2 \frac{\sin 2\pi rs}{2\pi rs} dr$$



Atomic scattering factor: $f \equiv \dfrac{E_a(s)}{E_e(s)}$

Example: Atomic scattering factor

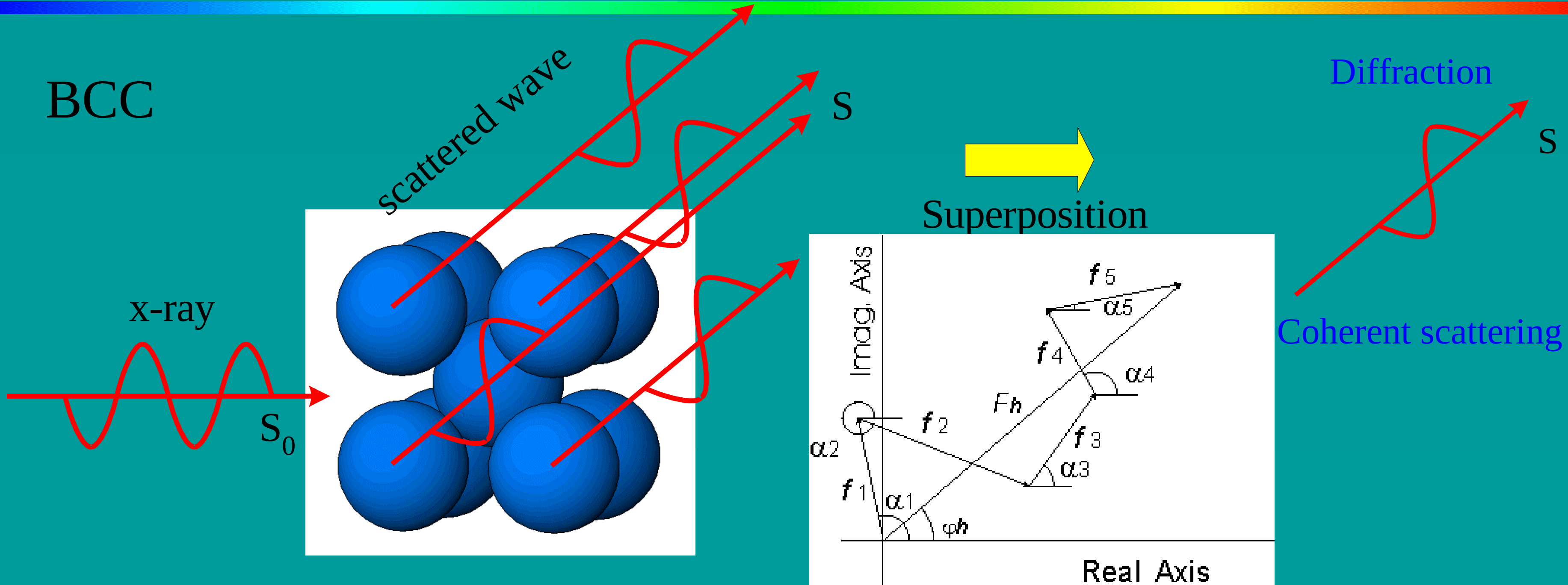
$$f = \frac{\text{amplitude of the wave scattered by an atom}}{\text{amplitude of the wave scattered by one electron}}$$



- "f " is expressed as a function of sinθ/λ as the interference depends on both λ and the scattering angle.

- "f" is equivalent to the atomic number at low angles, but it drops rapidly at higher sinθ/λ.

Scattering from one unit cell



$$E_{cell}(s) = E_e(s)\cdot\int_{cell}\rho(r)e^{2\pi i\vec{s}\cdot\vec{r}}d\vec{r}\ , \qquad \rho(\vec{r})=\sum_j\rho(\vec{r}-\vec{r}_j)$$

$$= E_e(s)\cdot\sum_j\Big[\int_{cell}\rho_j(\vec{r}-\vec{r}_j)e^{2\pi i\vec{s}\cdot(\vec{r}-\vec{r}_j)}d\vec{r}\Big]\cdot e^{2\pi i\vec{s}\cdot\vec{r}_j}$$

$$= E_e(s)\cdot\sum_j f_j e^{2\pi i(hx_j+ky_j+lz_j)}$$

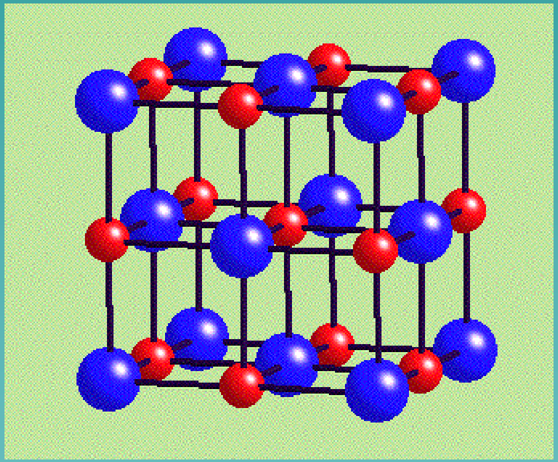
Structure factor 結構因子

$$|F_{hkl}| = \frac{\text{amplitude of the wave scattered by all the atoms in one unit cell}}{\text{amplitude of the wave scattered by one electron}}$$

$$F_{hkl} = \frac{E_{cell}(s)}{E_e(s)} = \sum_{cell} \rho(r) e^{2\pi i \vec{s}\cdot\vec{r}} d\vec{r}$$

$$= \sum_j f_j e^{2\pi i (hx_j + ky_j + lz_j)}$$

NaCl



One unit cell contains 4(Na^+Cl^-)

Kinematical theory 靜力

$$I = |F_{hkl}|^2 \cdot p \cdot \left(\frac{1+\cos^2 2\theta}{\sin^2\theta \cdot \cos\theta}\right) \cdot A(\theta) \cdot e^{-2M}$$

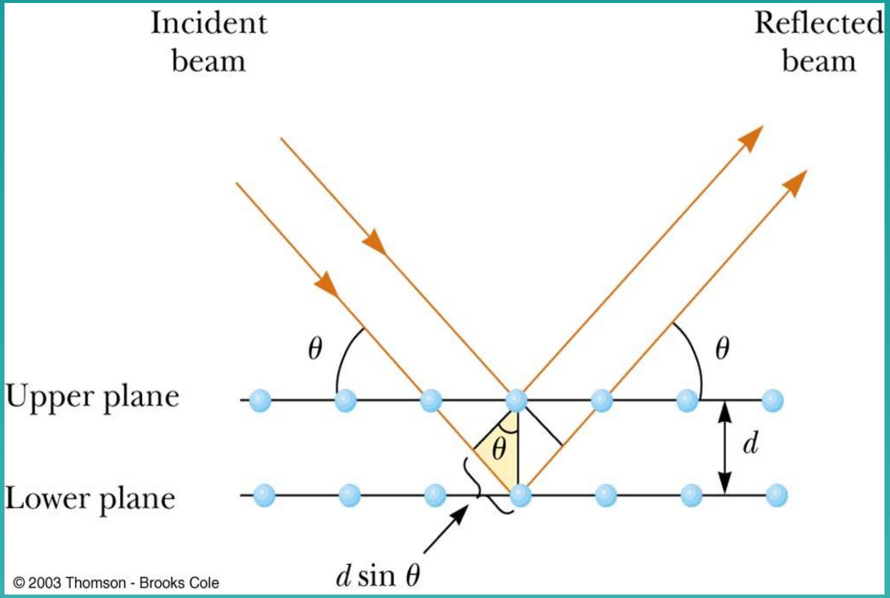
Dynamical theory 動力

$$I = \frac{8}{3\pi}\left(\frac{e^2}{mc^2}\right)\frac{N\lambda^2 |F_{hkl}|}{\pi \sin 2\theta}\left(\frac{1+|\cos 2\theta|}{2}\right)$$

Bragg's Law 布拉格定律

- The beam reflected from the lower surface travels farther than the one reflected from the upper surface
- If the path difference equals some integral multiple of the wavelength, constructive interference occurs
- *Bragg's Law* gives the conditions for constructive interference

Perfect Crystal = 3D Grating



$$2d\sin\theta = n\lambda$$

n=1, 2, 3, …

d: Lattice spacing

λ: Wavelength of x-ray

θ: Bragg angle

應用
Applications

Applications of X-ray Diffraction

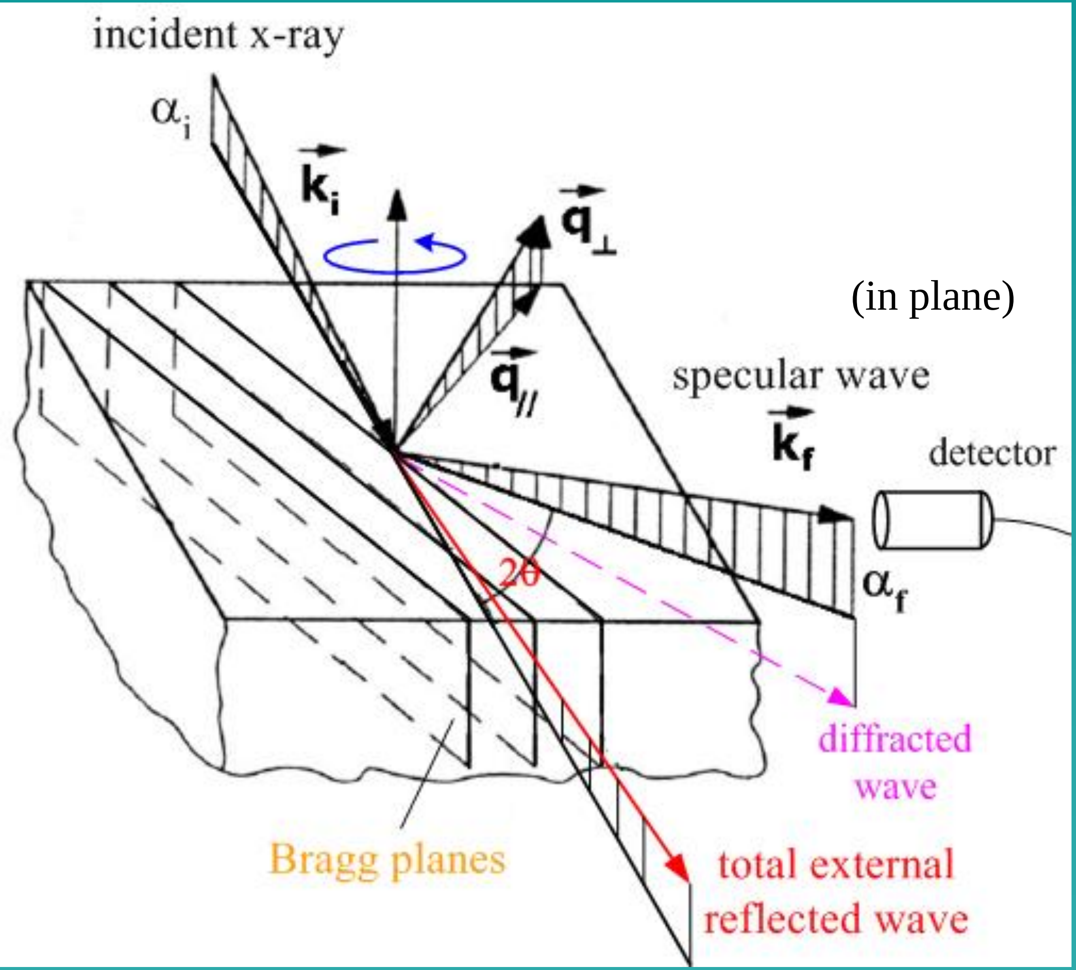
- **Biological and chemical 3D molecular structure determination (SCD)**
- **Qualitative and quantitative crystalline phase composition analysis (XRPD)**
- **Material structure analysis (XRD, HRXRD, XRR, μ-XRD, SAXS)**
  - crystallite size / particle size in the nm range
  - microstrain
  - residual stress / fatigue stress
  - texture / preferred orientation
  - thin films and multilayers: thickness, layer sequence, density, surface and interface roughness
  - Nanostructure analysis (particle shape, size and orientation)

Techniques used for X-ray Diffraction

- **X-ray powder diffraction (XRPD)**
- **High resolution X-ray diffraction (HRXRD)**
- **Single crystal diffraction (SCD)**
- **Small angle X-ray scattering (SAXS)**

- **X-ray reflectometry (XRR)**
- **Grazing incidence diffraction (GID)**
- **In-plane grazing incidence diffraction (IPGID)**
- **X-ray resonant diffraction**
- **X-ray multiple diffraction**

Grazing (Glancing) Incidence X-Ray Diffraction (GIXD)



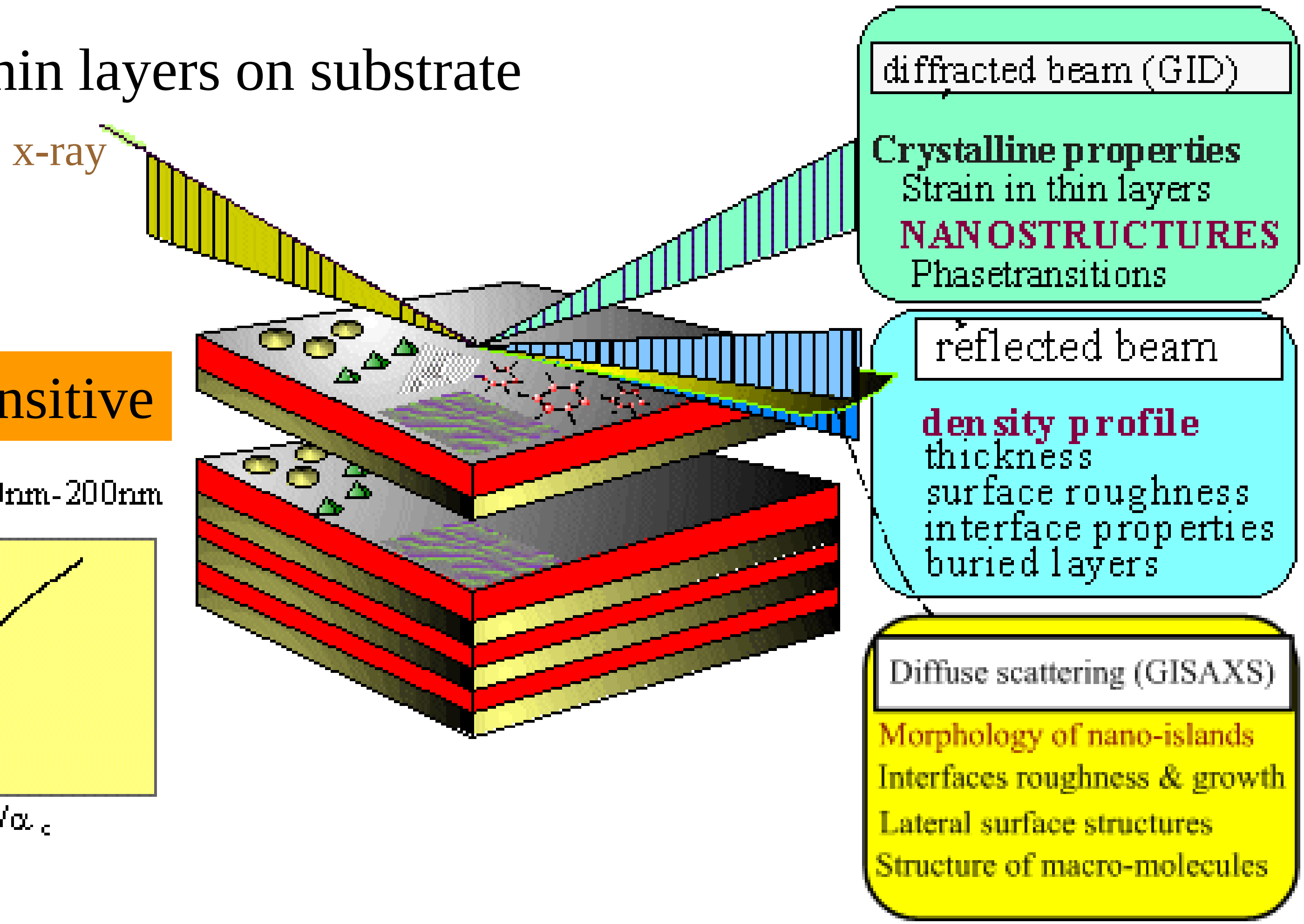
When the incident beam close to or below the critical angle for total external reflection, a Bragg reflection is excited from planes perpendicular to the surface.

Greatly enhanced surface sensitivity

Information from Grazing Incidence X-rays

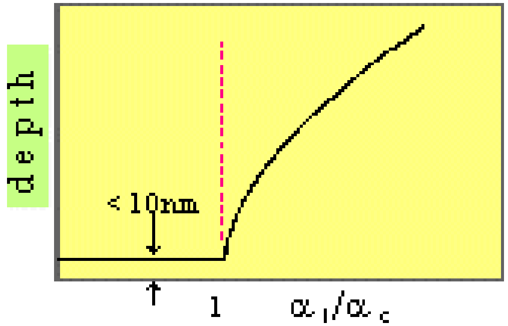
X-ray methods at grazing incidence (GID, GISAXS,…)

Structure of thin layers on substrate

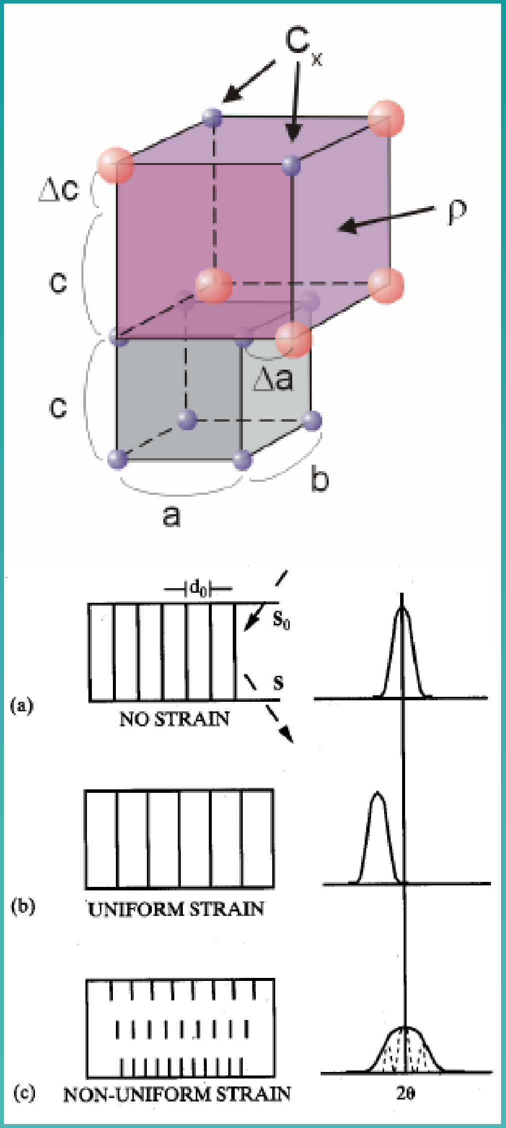


Surface sensitive

depth resolution 10nm-200nm



Strain



crystalline diffraction line

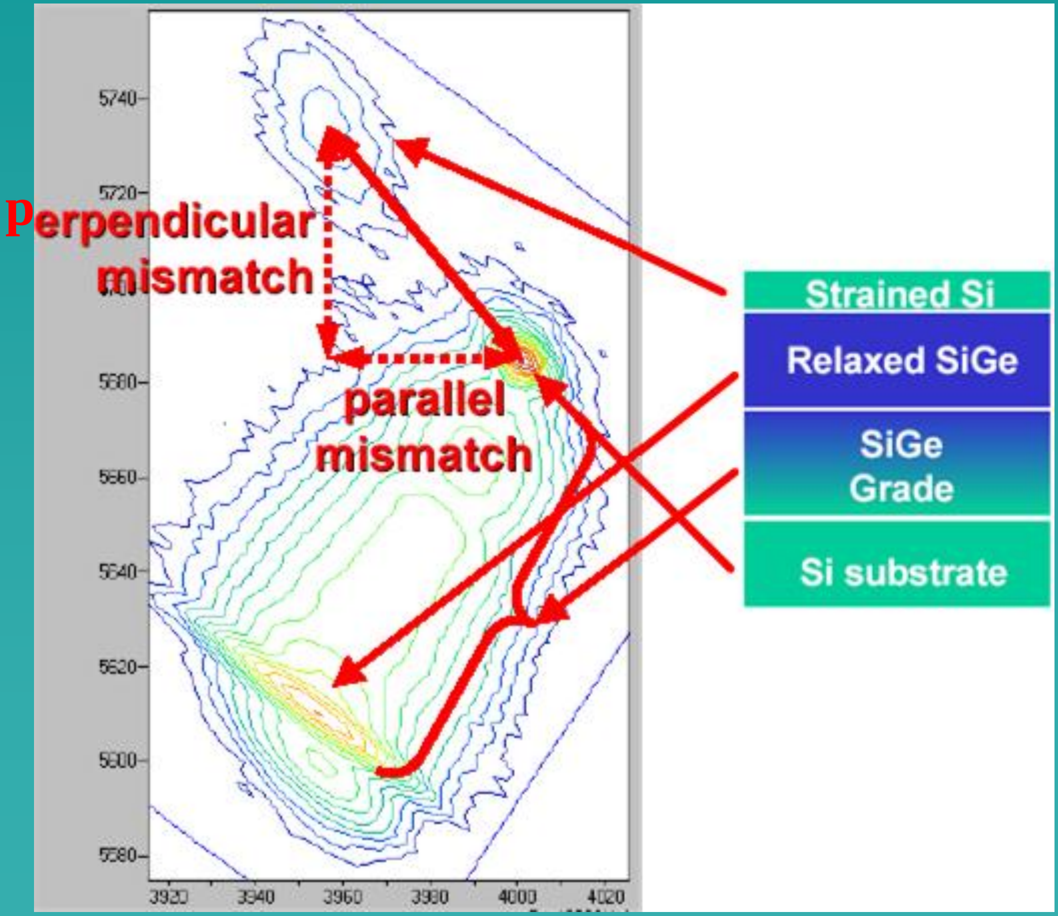
- **Δa/a**
  Mismatch (or strain) in lateral (in-plane, parallel) direction.
- **Δc/c**
  Mismatch (or strain) in normal (vertical, perpendicular) direction.
- **R**
  Lattice relaxation degree.
- **ρ**
  Mass density
- c_x
  Concentration for ternary solid solution
- c_y
  Concentration for quaternary solid solution

In a material there may be strains that vary from grain to grain or within a grain (microtrains) due to the local environment and there may also be a uniform strain due to an external load (macrostrain)

Differential Bragg's law

$$\Delta 2\theta = -\frac{\Delta d}{d}\tan\theta$$

How to measure strain



Horizontal offset gives parallel lattice constant

Vertical offset gives perpendicular lattice constant

Combining the lattice constant information gives the parallel and perpendicular strain

Basic concepts of reflectivity

Specular x-ray reflectometry - characterize e^- density profile normal to the interface

Refracive index for x-ray:

$n = 1 - \delta + i\beta$, less than 1, for X-ray!

$\delta = r_0 \rho_0 \lambda^2 / 2\pi$ (10^{-5} to 10^{-6})

and β - absorbtion, $\beta = \mu\lambda/4\pi$

r_0 - clasical electron radius

ρ_0 - electron density

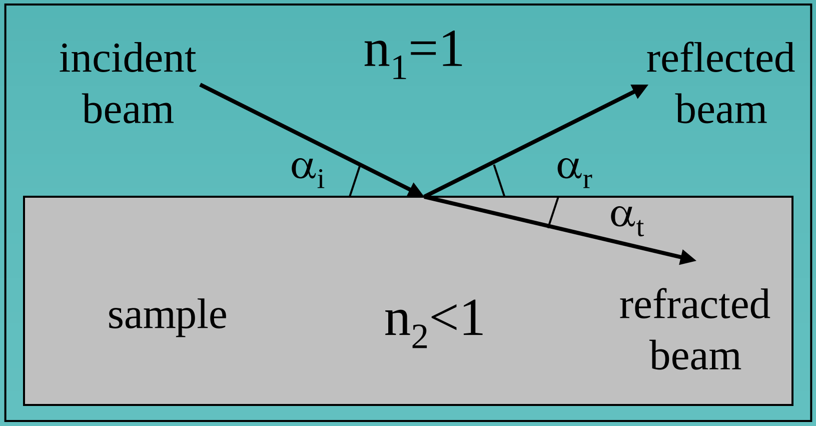
μ - mass absorption coefficient

Snell's law:

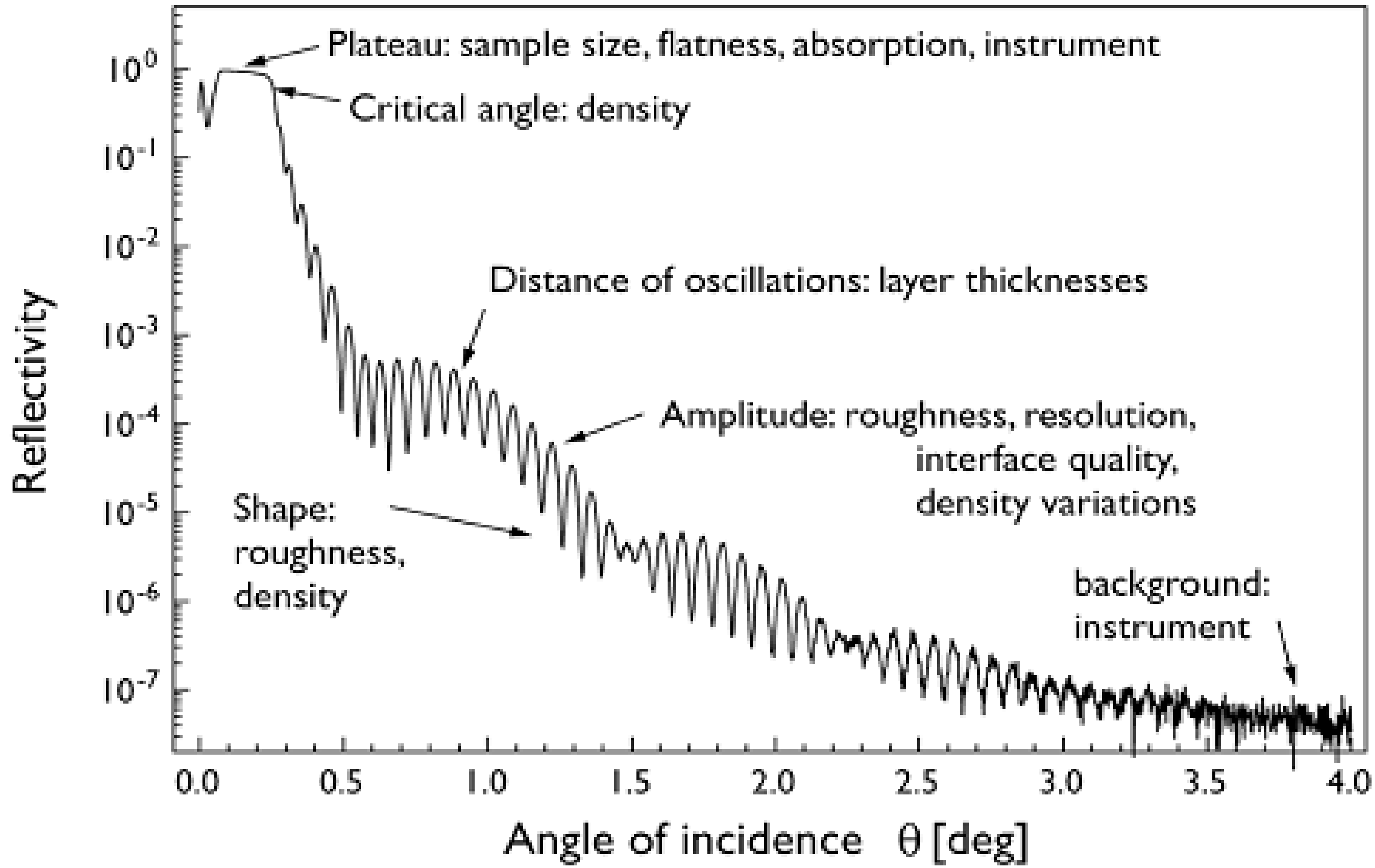
$n_1 \cos \alpha_i = n_2 \cos \alpha_t$

α_c (α_i for $\alpha_t = 0$) = $(2\delta)^{1/2}$

$\alpha_c \sim 0.1 - 0.6^\circ$ for $\lambda = 1.5$Å



The Information Derived from a Reflectivity Curve

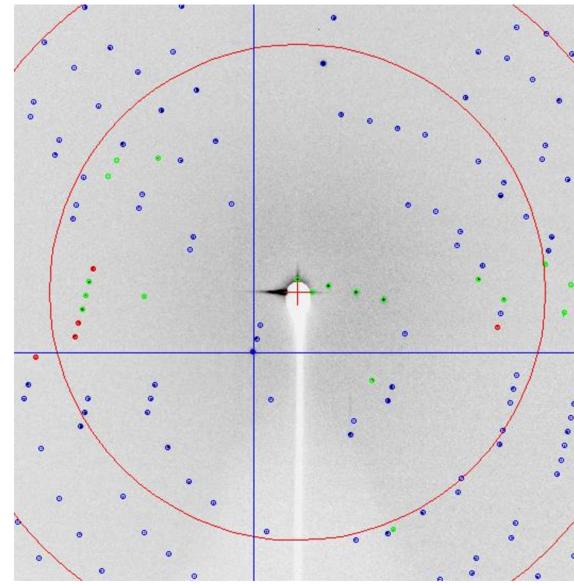


X-ray crystallography X光結晶學

1.Crystallization

2.Data collection

3.Phase determination



6.Structure

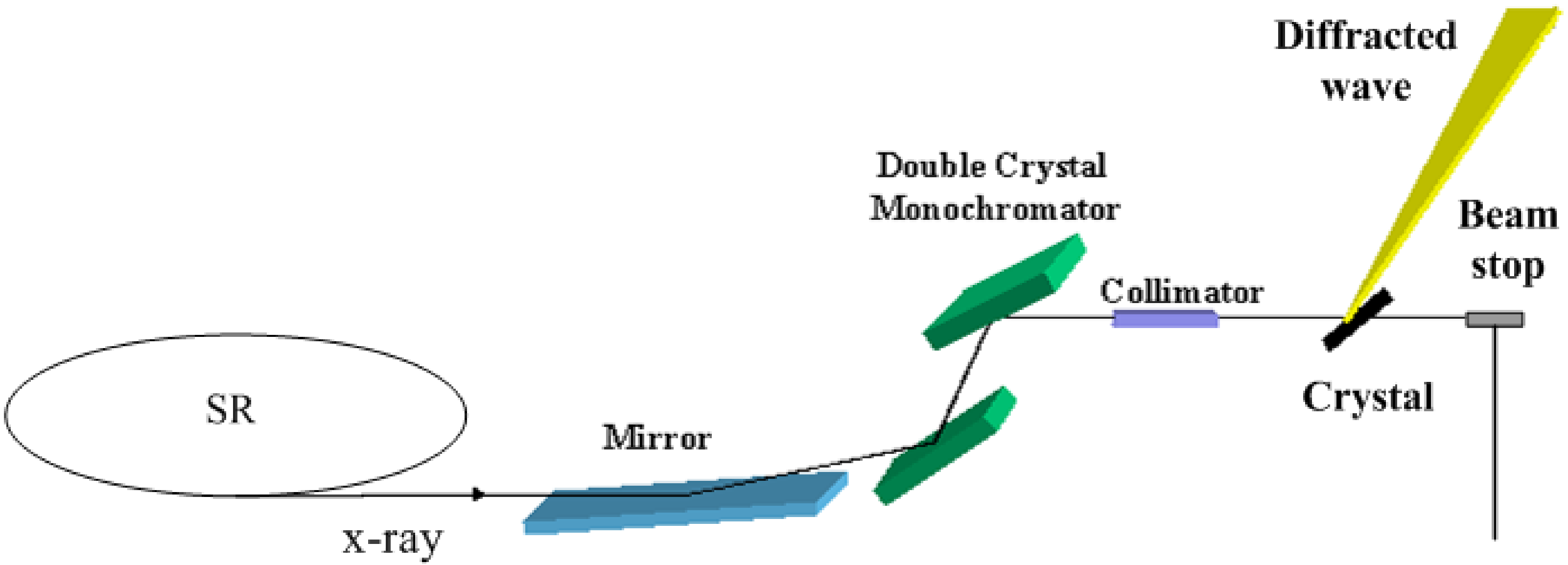
$$I \propto |F_{hkl}|^2$$

$$F_{hkl} = |F_{hkl}| e^{i\alpha_{hkl}}$$

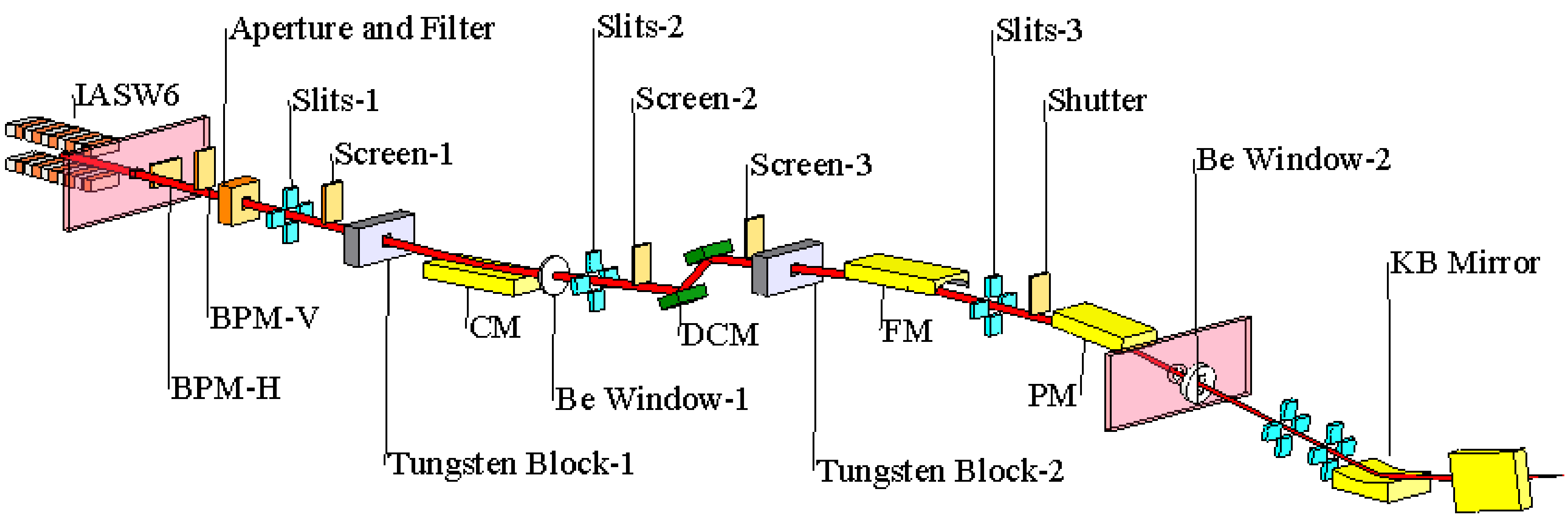
4.Calculation & interpretation of electron density map

5.Refinement of the molecular model

Beamline Setup

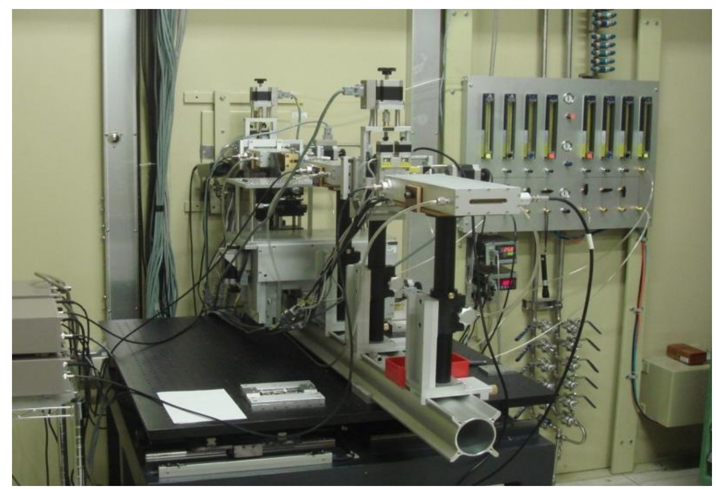


X-ray Scattering BL07A (NTHU, Tamkang U., T3)

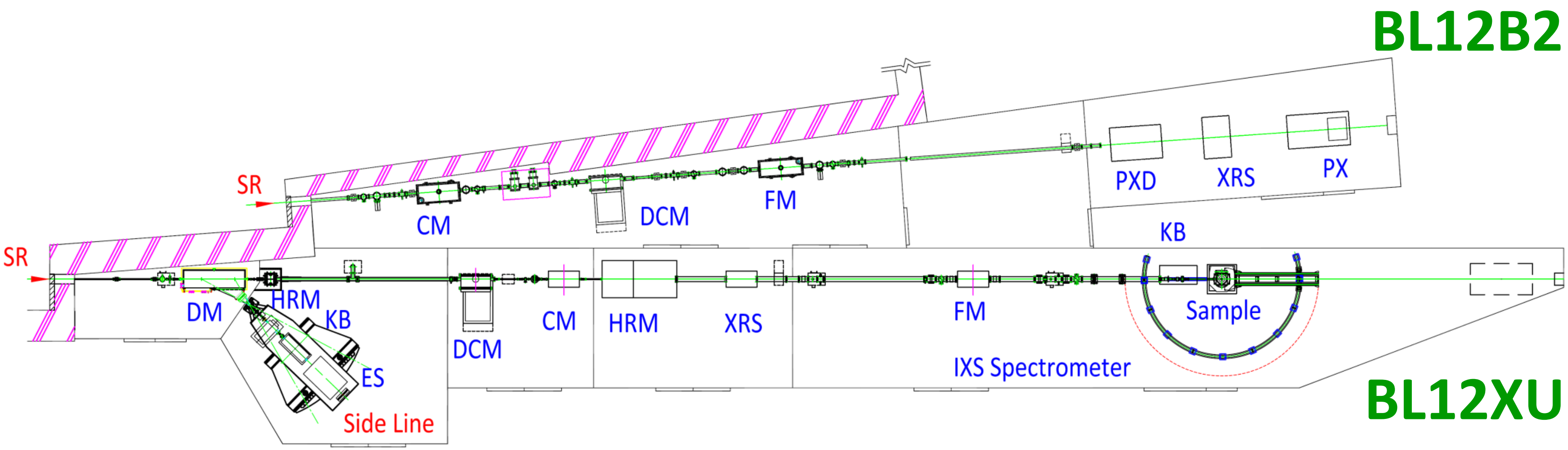


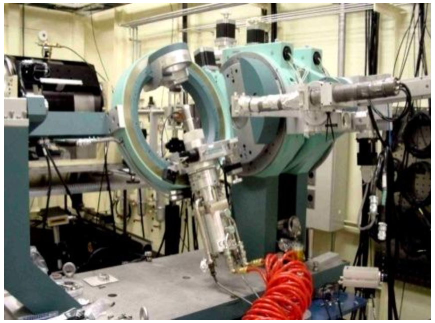
X-ray scattering/diffraction station

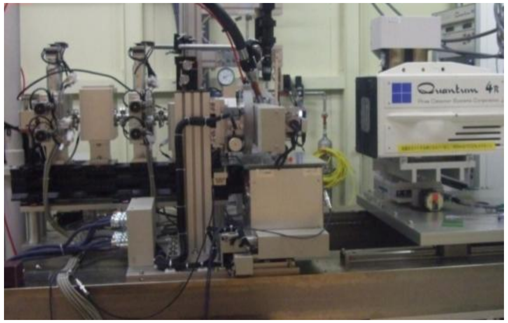
X-ray absorption station



SPring-8 Taiwan Beamlines



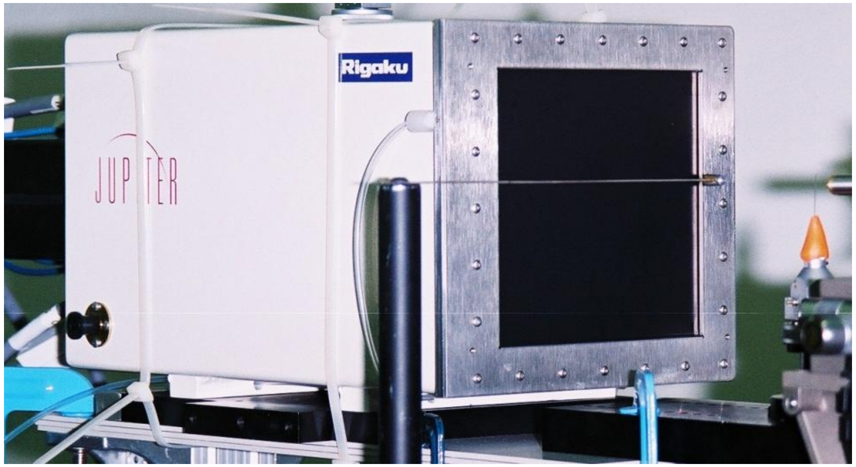




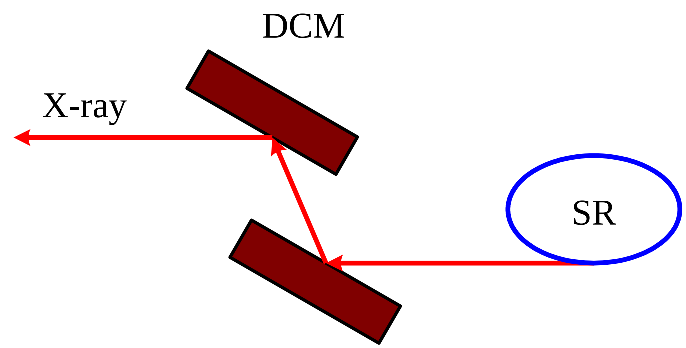
10Y review & 5Y contract renewal (2010/2/24)

Data Collection

Charge Couple Device (CCD)



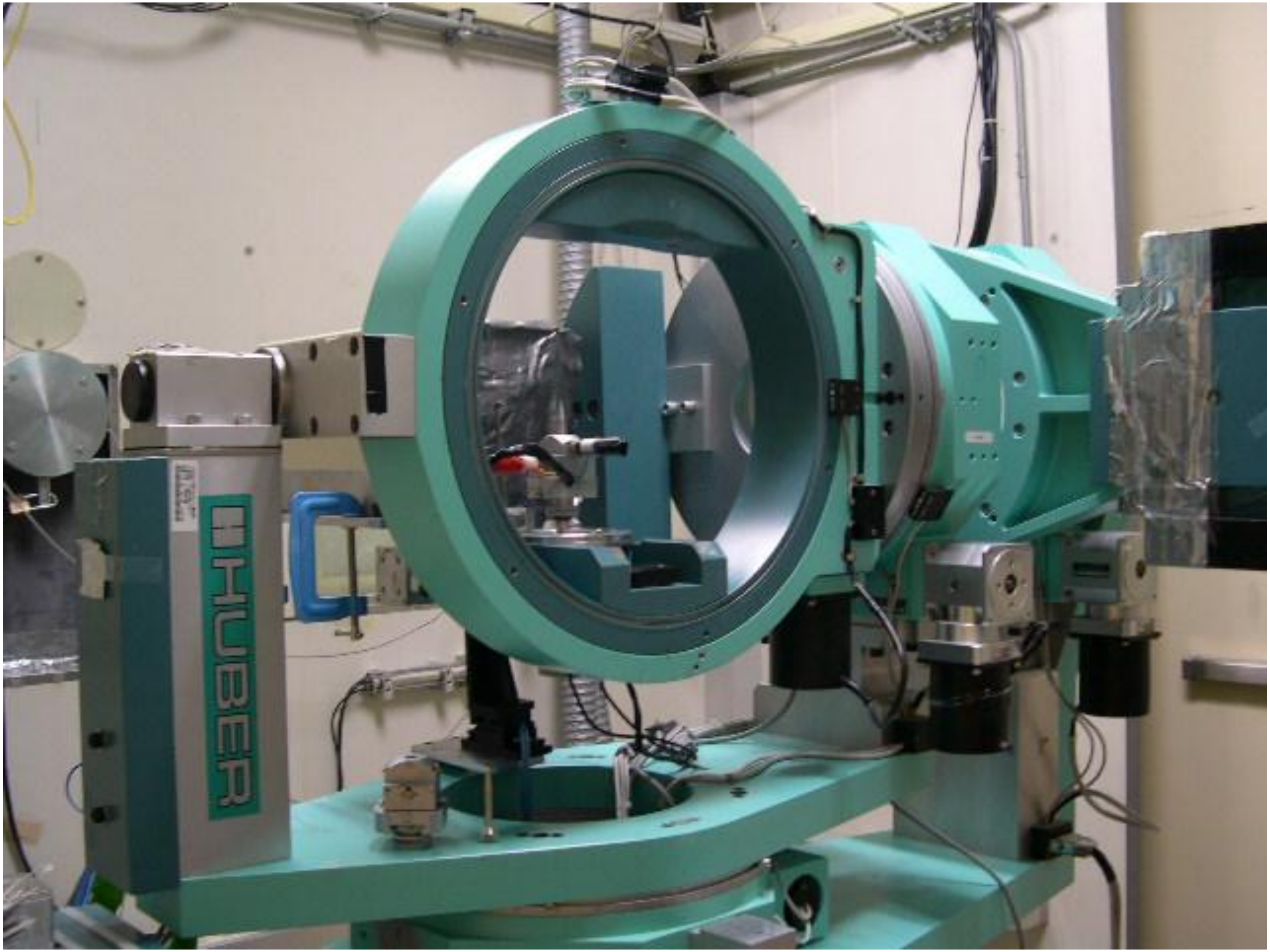
Lysozyme



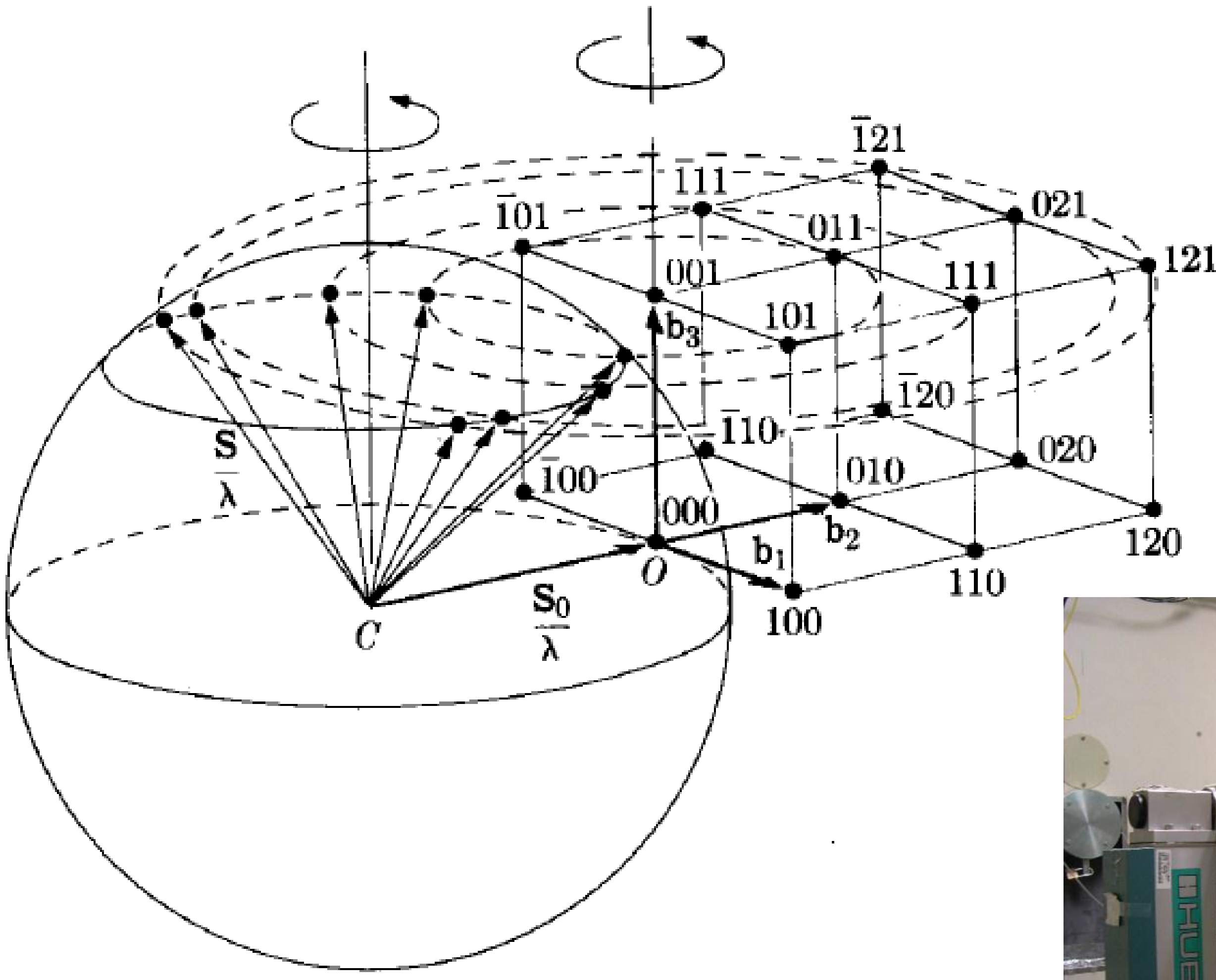
Control PC system

8C diffractometer

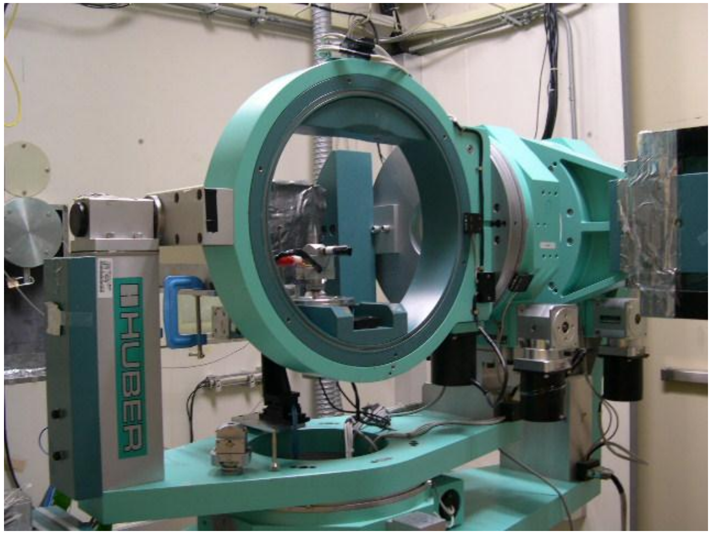
8C diffractometer 八環繞射儀器



Data collection method: Rotation method



Ewald sphere



Diffraction Image of Lsozyme

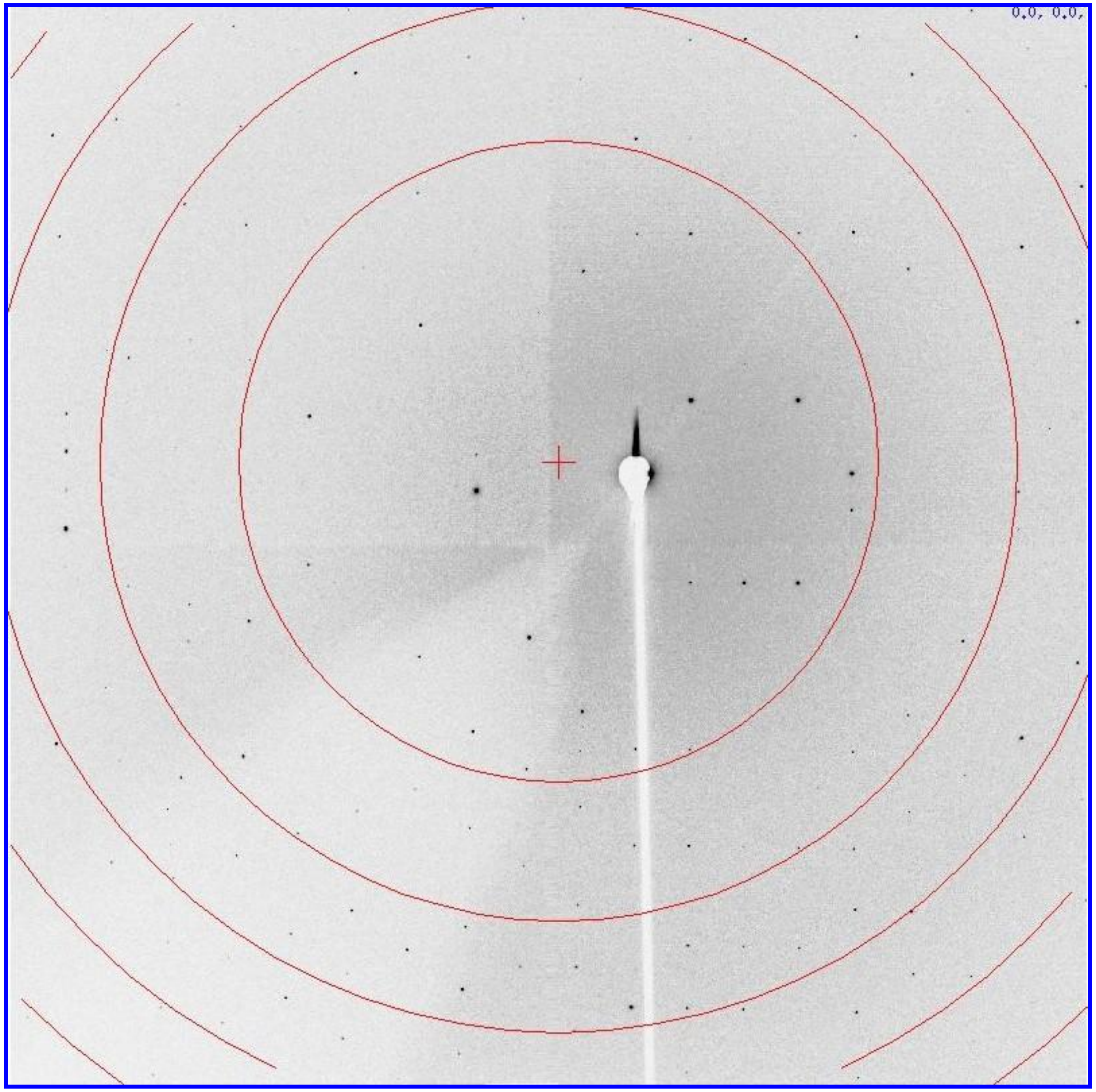


Photo: MRC Laboratory of Molecular Biology

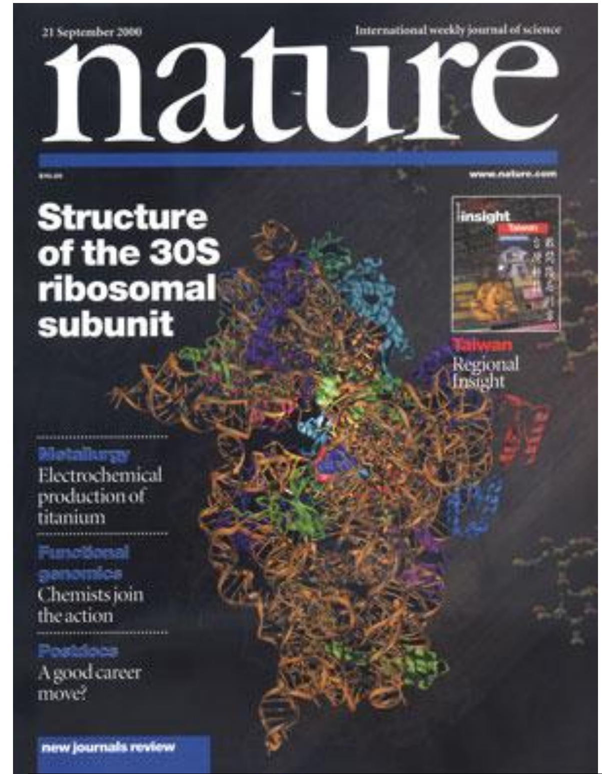
Credits: Michael Marsland/Yale University

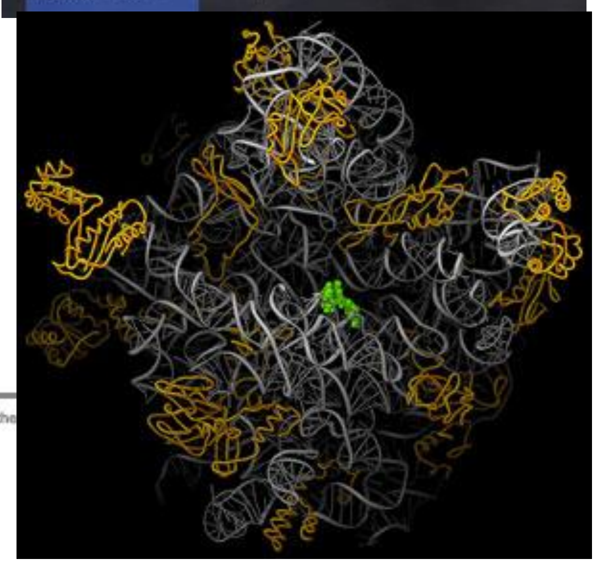
Credits: Micheline Pelletier/Corbis

Venkatraman Ramakrishnan	Thomas A. Steitz	Ada E. Yonath
1/3 of the prize	1/3 of the prize	1/3 of the prize
United Kingdom	USA	Israel
MRC Laboratory of Molecular Biology Cambridge, United Kingdom	Yale University New Haven, CT, USA; Howard Hughes Medical Institute	Weizmann Institute of Science Rehovot, Israel
b. 1952 (in Chidambaram, Tamil Nadu, India)	b. 1940	b. 1939

Titles, data and places given above refer to the time of the award.

Source: Nobel Prize website





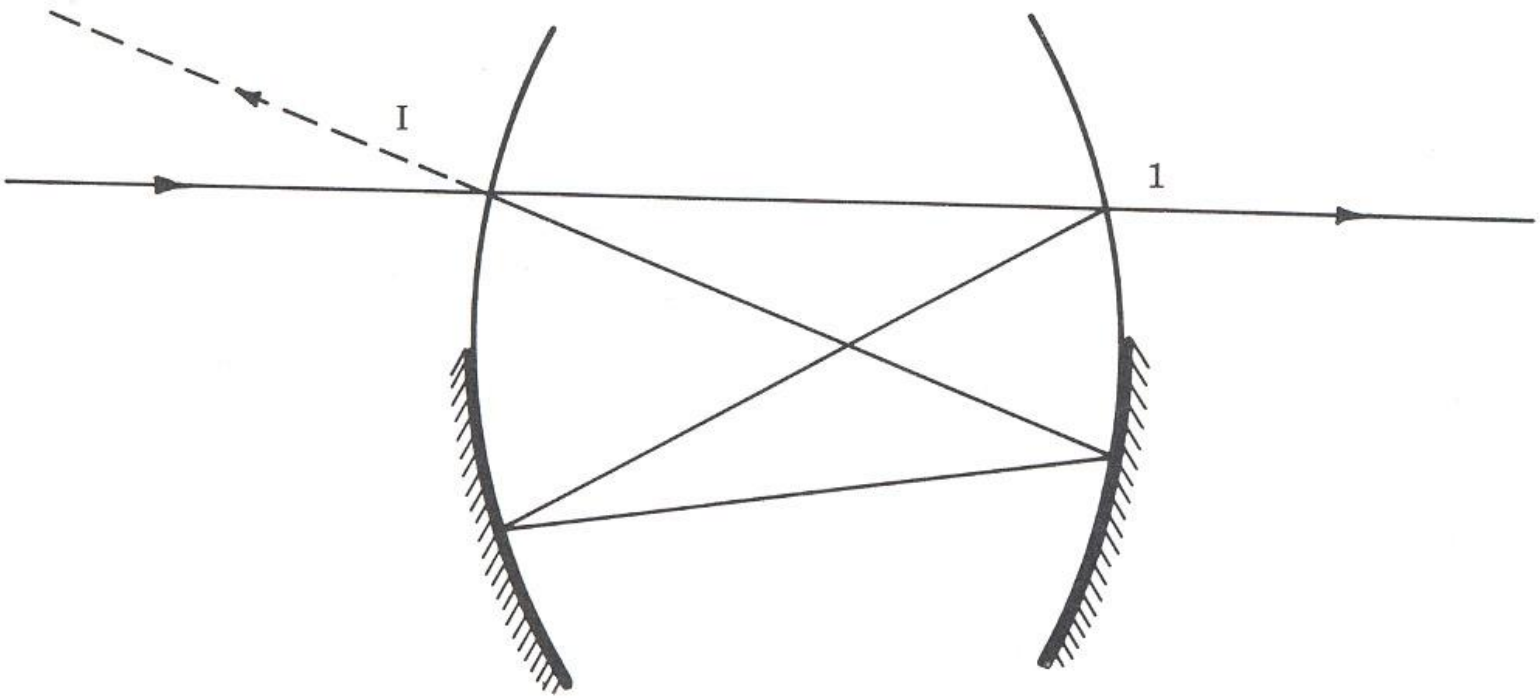
Source: NSLS website

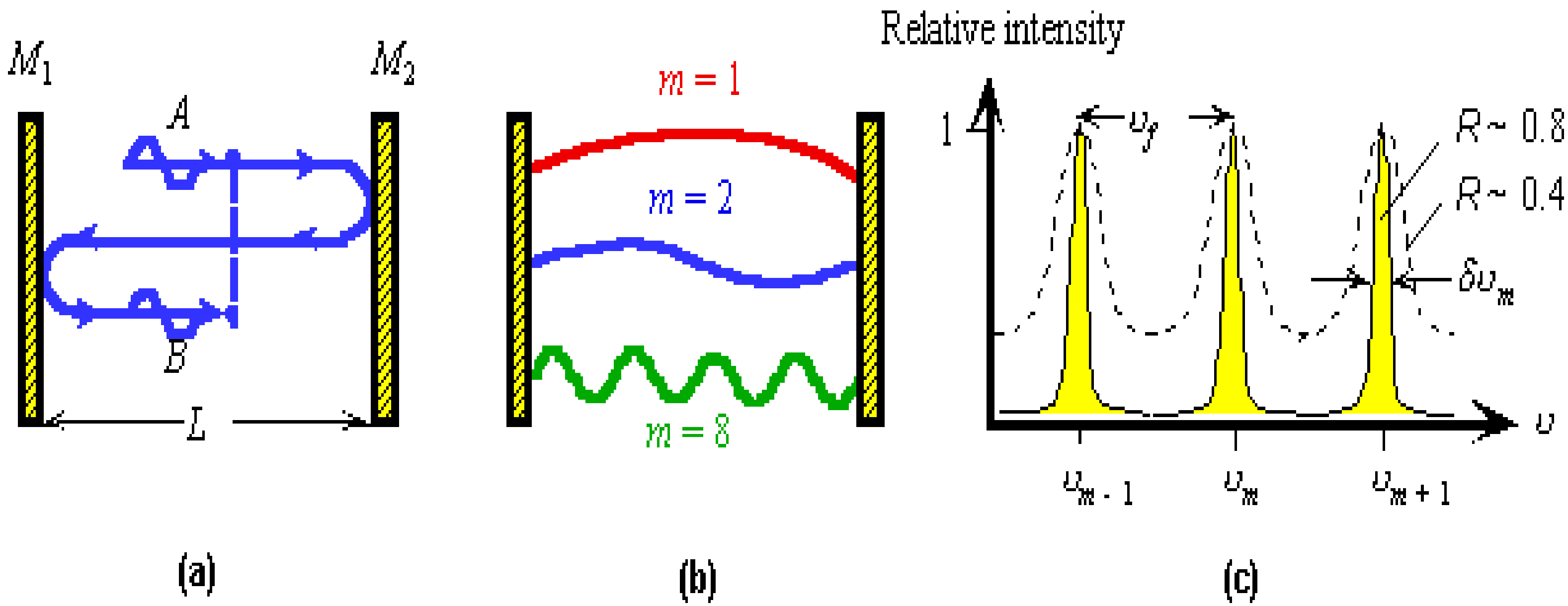
Realization of X-Ray Fabry-Perot Cavity: A Synchrotron Diffraction Experiment

X光共振腔--X光繞射實驗

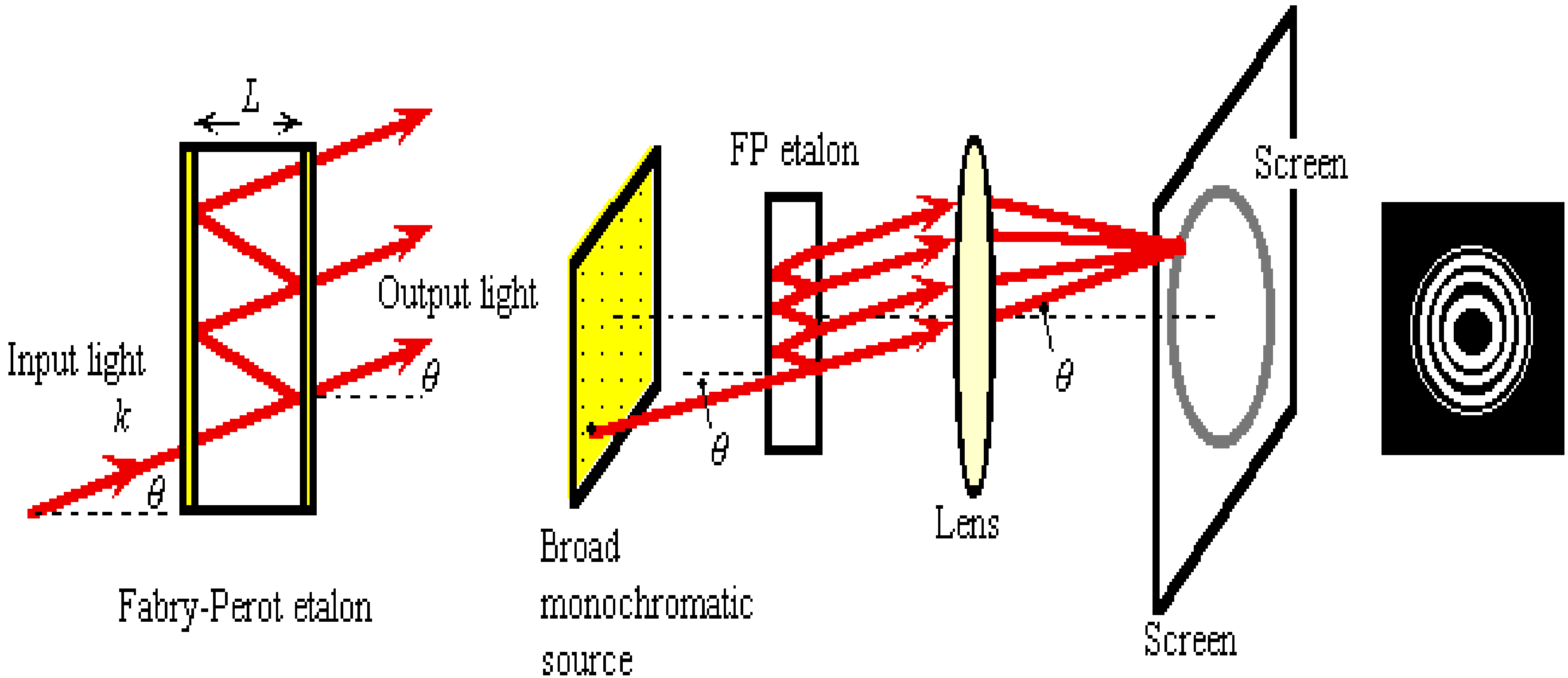
NTHU, NSRRC, SPring8/Riken

Optical Fabry-Parot Interferometer



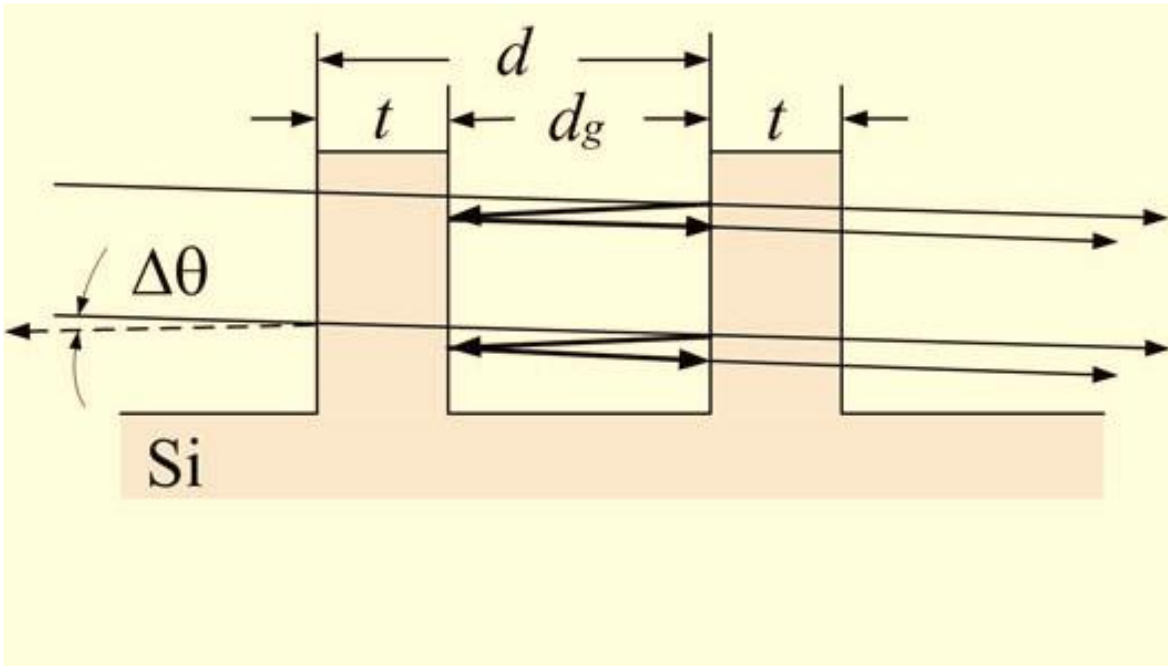


Schematic illustration of the Fabry-Perot optical cavity and its properties. (a) Reflected waves interfere. (b) Only standing EM waves, *modes*, of certain wavelengths are allowed in the cavity. (c) Intensity vs. frequency for various modes. *R* is mirror reflectance and lower *R* means higher loss from the cavity.



Fabry-Perot optical resonator and the Fabry-Perot interferometer (schematic)

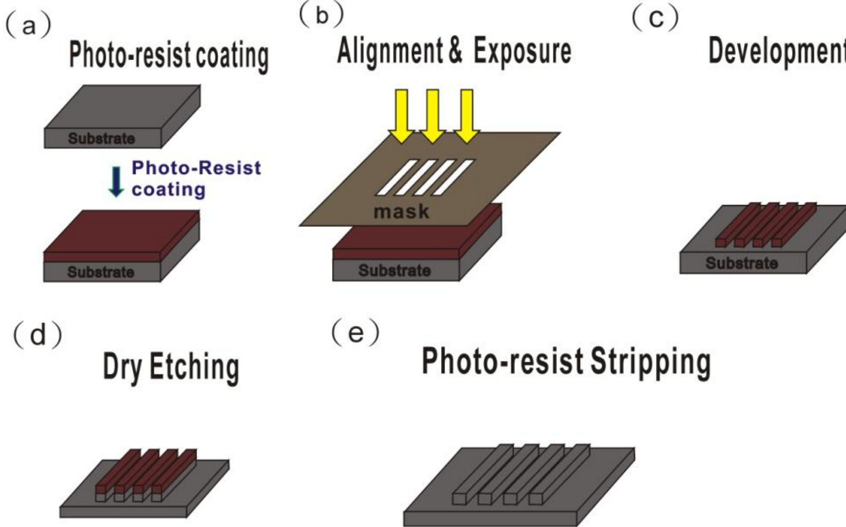
X-ray Fabry-Perot resonator

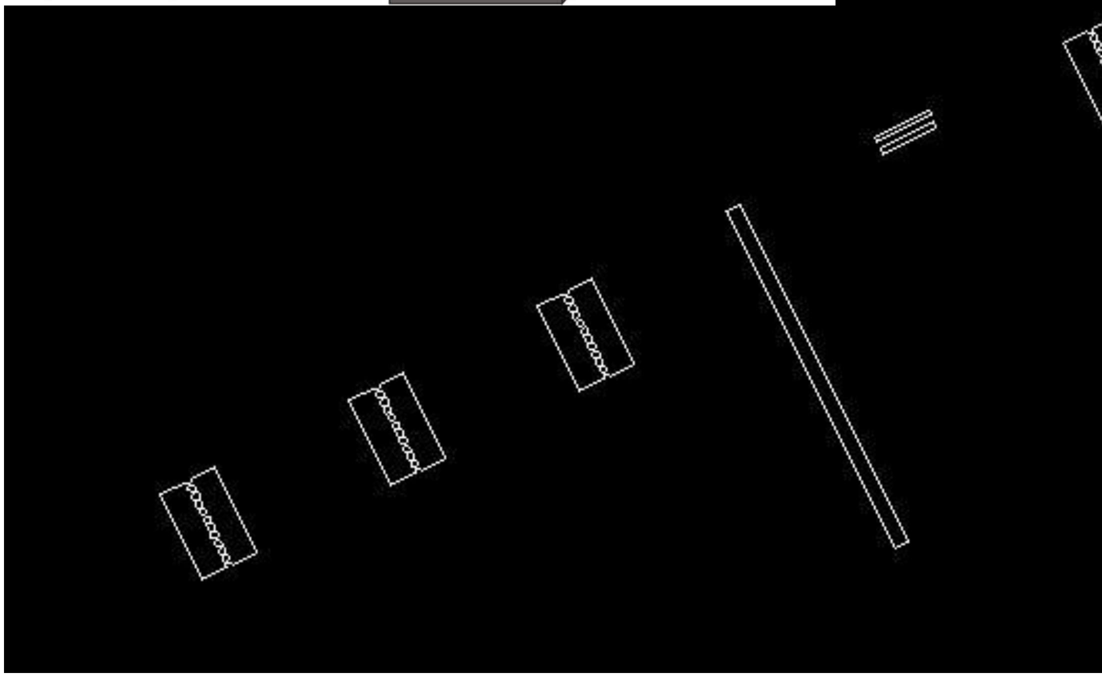


背向反射(back reflection)

Bragg angle=90 deg.

微電子蝕刻術 (lithography)





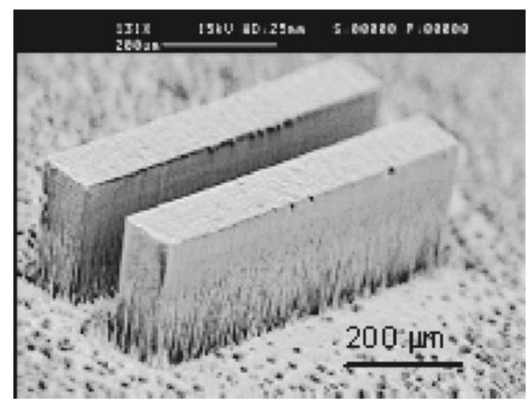
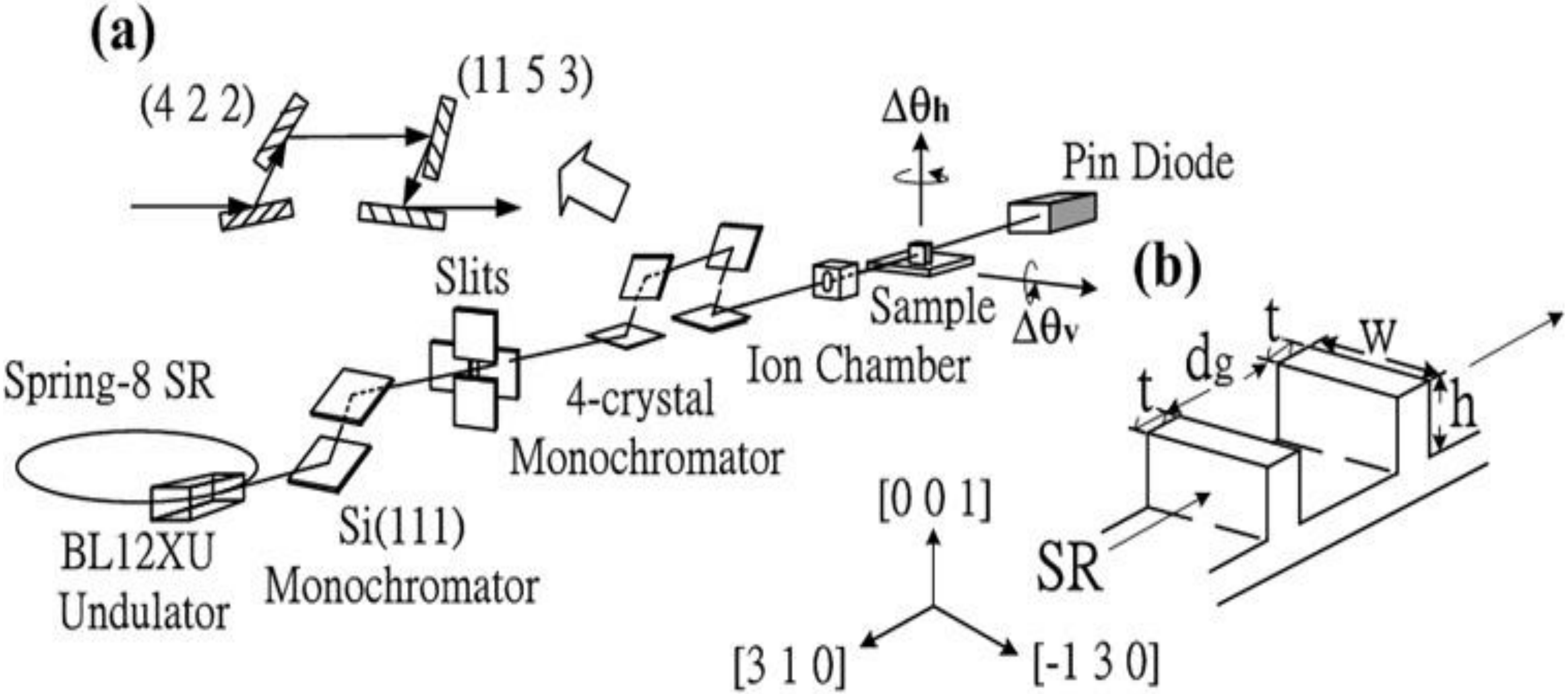


FIG. 1. A SEM photograph of a thick two-plate (100/100) x-ray Fabry-Pérot cavity of silicon. The width of the crystal plate is 800 μm, the height is 200 μm, and the thickness is 100 μm. The direction normal to the substrate plane is [001] and that perpendicular to the two crystal plates is [310].

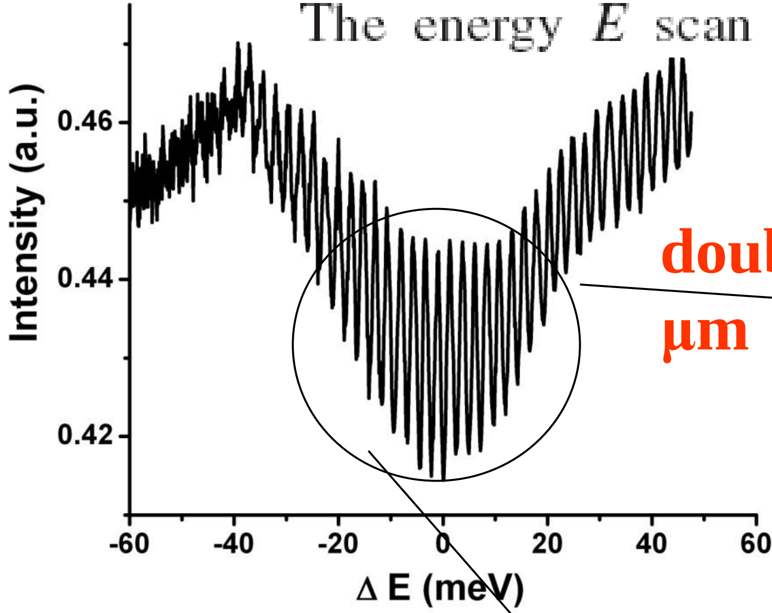
Experimental set-up



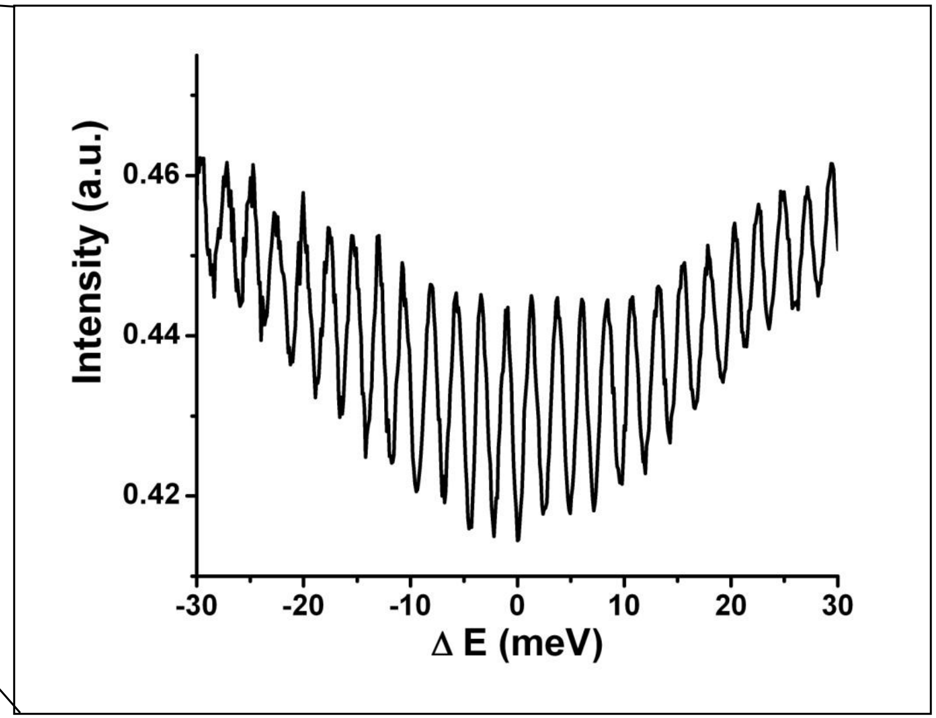
Si (12 4 0) back reflection

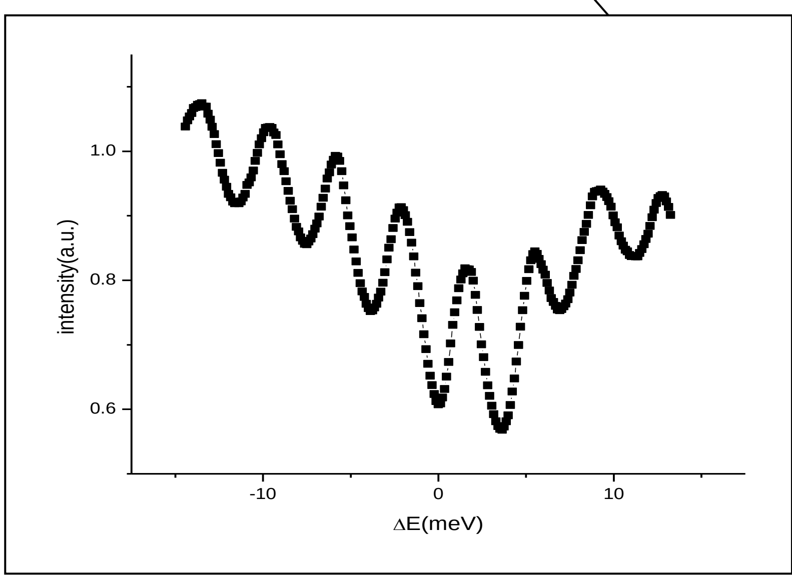
for **E=14.4388 keV** (0.8588 A)

The energy E scan of the forward-transmitted (000)



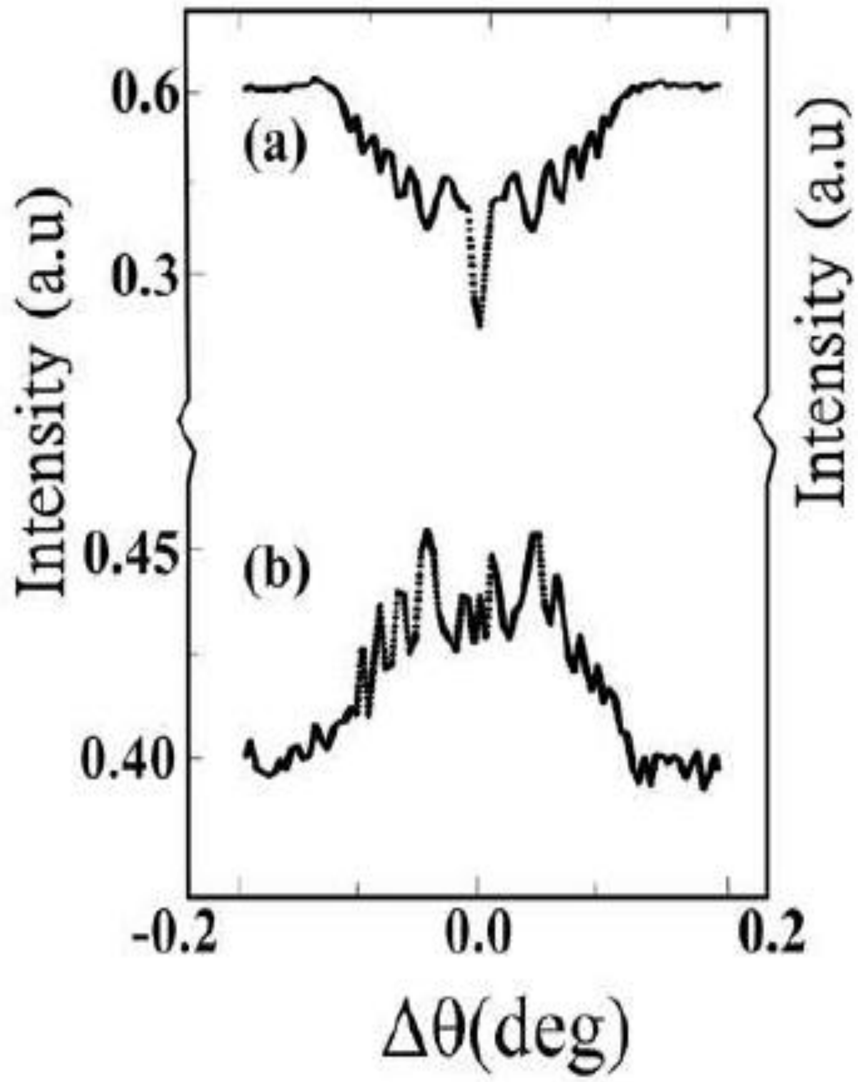
double thin plates, t = 100μm dg = 150 μm





double thinner plates, t = 70 μm dg = 100 μm

Δθ- scans at ΔE = 9 meV
The Δθ-scan at 0.002 deg./step



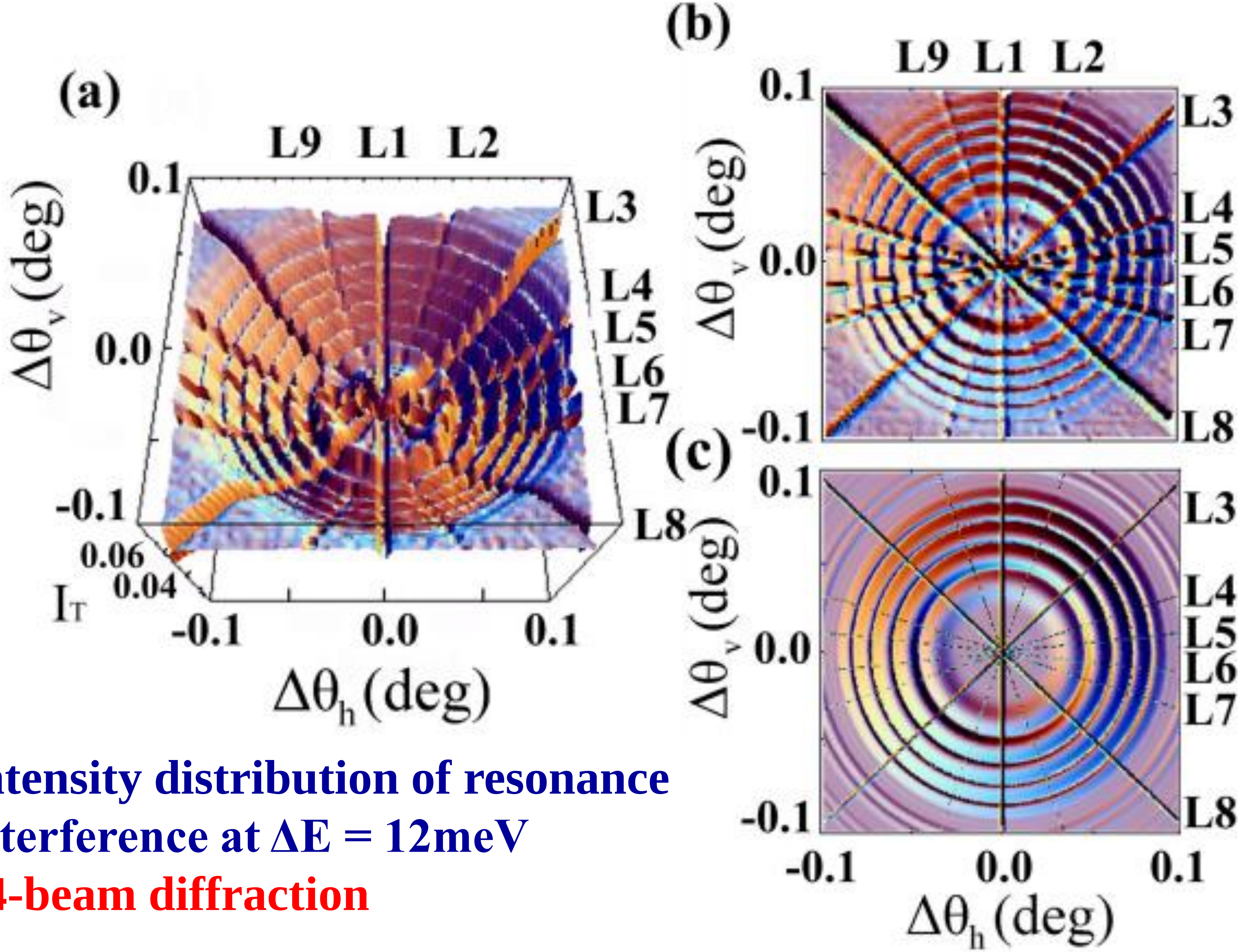
$\Delta E = 0.36 meV$

$\Delta E/E = 2.5 * 10^{-8}$ at 14.4388 keV (0.8588 A)

(a) Forward-transmitted (0 0 0) beam

(b) Back-reflected **(12 4 0)** beam

Silicon crystal



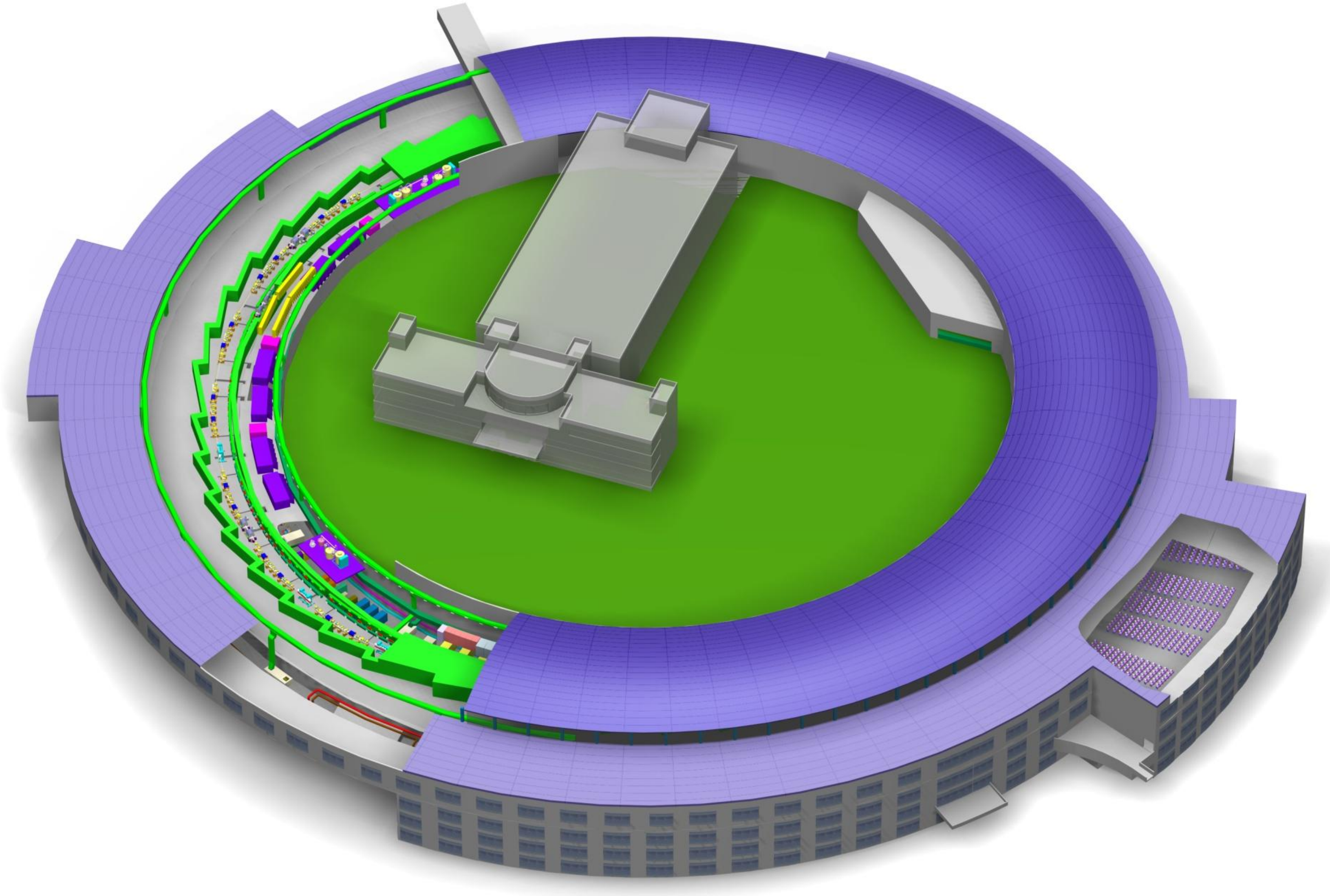
Intensity distribution of resonance interference at ΔE = 12meV

24-beam diffraction

Collaboration: NTHU, NSRRC, SP-8/RIKEN

S.-L. Chang, et al *Phys. Rev. Lett*. **94**, 174801 (2005).

台灣光子源計畫
Taiwan Photon Source (TPS) Project



台灣光子源 Taiwan Photon Source (TPS)

3D Aerial View of NSRRC

Full capacity: 48 ports

Progress of Civil Construction

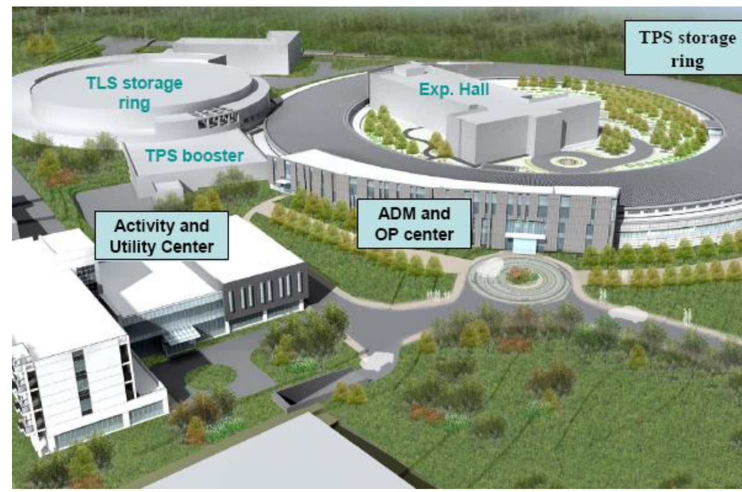
TLS交界處拆除及開挖

深開挖處植入土釘

儲存環館第一、二區完成土層開挖

儲存環館鋼筋綁紮準備灌漿

台灣光子源興建工程動土典禮 2010. 2. 7



D棟地下二層開挖整地

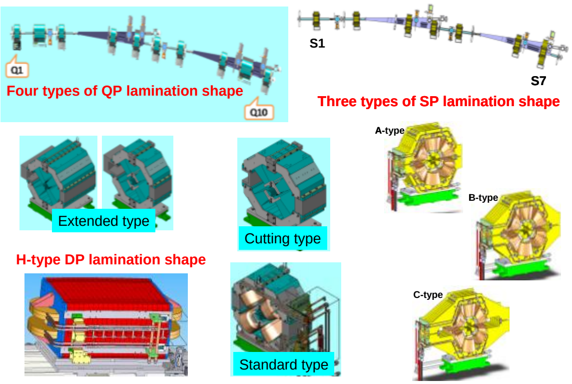
地下二層佈植鋼筋灌漿

地下二層植筋模板準備灌漿

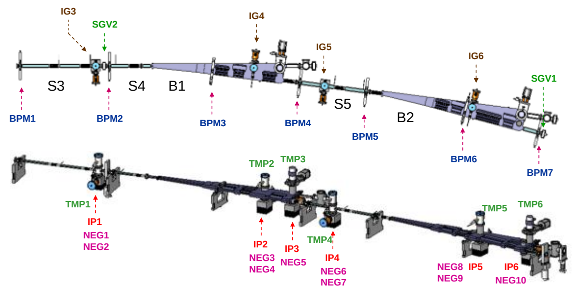
地下一層佈植鋼筋準備灌漿

TPS Accelerator Design and Prototype

二極、四極與六極磁鐵



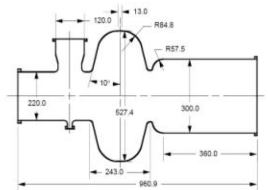
真空系統設計與射束診斷安排



超導高頻共振腔

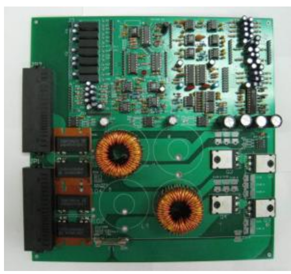
KEKB Type SRF Module

- Installed at KEKB (508 MHz) and BECP-II/IHEP (500 MHz)



修正磁鐵電源供應器原型

(與工研院合作開發)



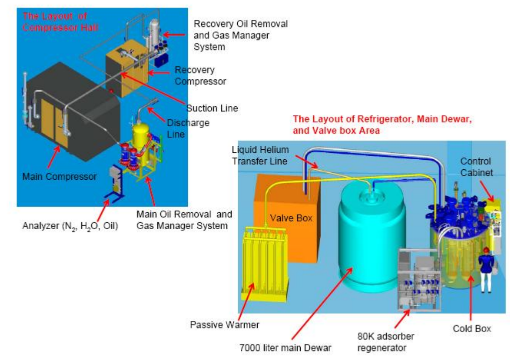
Specification

Max. volt/cur.:	±50V/±10A
Current ripple:	10 ppm
Short term stability:	5 ppm
Long-term stability:	10 ppm

Total 750 units to be fabricated by local company

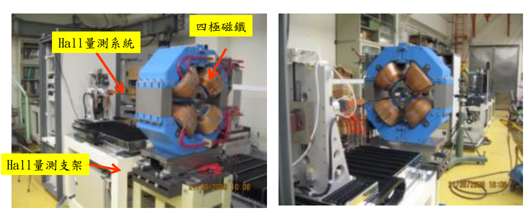
屏蔽牆內儲存環與增能環結構

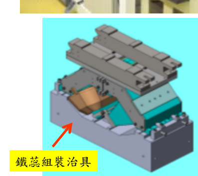
700 W液氦低溫系統配置

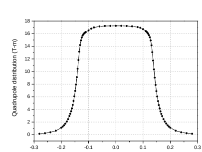


TPS儲存環1/24段實體照片

四極磁鐵原型及量測平台







沿軸向四極鐵磁場強度測試

- 四極成分達設計值
- 八、十二極分量超出規格
- 工程精度需提昇(底座等)
- 品質需強化(線圈溫升)

潔淨室無油加工鋁質二極真空腔

3D dipole Al chamber machining

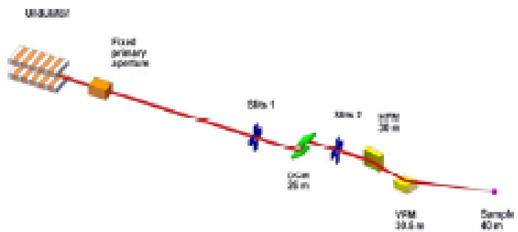
1. In clean room
2. Oil free environment
3. High precision on profile

TPS Phase I Beamlines

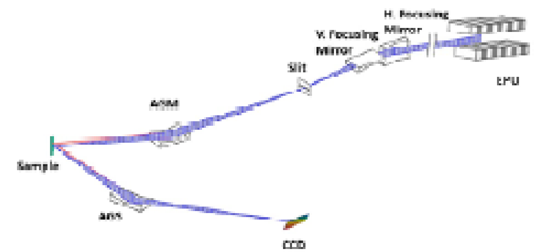
- *μ-focus macromolecular crystallography* (2013)
  *(*微聚焦巨分子結晶學光束線*)*
- *High resolution inelastic soft-x-ray scattering* (2013)
  *(*高解析非彈性軟X光散射學光束線*)*
- *Sub-μ soft x-ray photoelectron & fluorescence emission* (2013)
  (次微米軟X光能譜學光束線)
- *Coherent x-ray scattering (SAXS/XPCS)* (2014)
  *(*軟物質小角度散射學光束線*)*
- *Sub-μ x-ray diffraction* (2014)
  *(*次微米繞射光束線光束線*)*
- *Nano-probe* (2014)
  *(*奈米探針光束線*)*
- *Temporal coherent x-ray scattering* (2014)
  *(*時間同調性散射光束線*)*

TPS首期7條光束線之概念設計圖

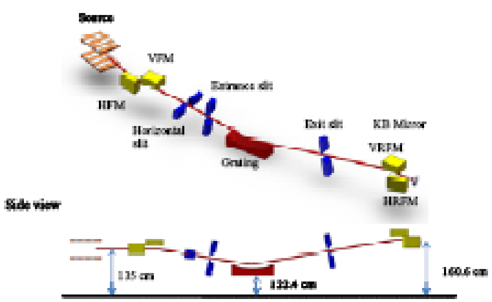
微聚焦巨分子結晶學光束線
(μ-focus macromolecular crystallography)



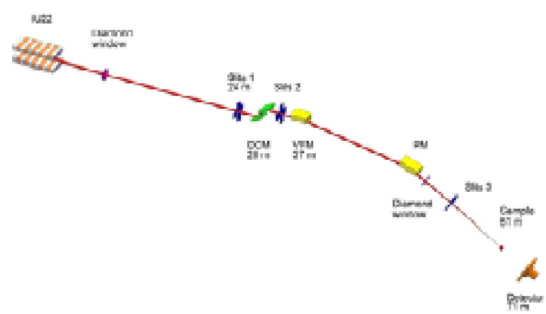
高解析非彈性軟X光散射學光束線
(High resolution Inelastic soft-x-ray scattering)



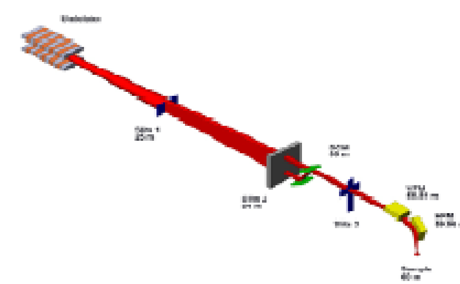
次微米軟X光能譜學光束線
(Sub- μ soft x-ray photoelectron & fluorescence emission)



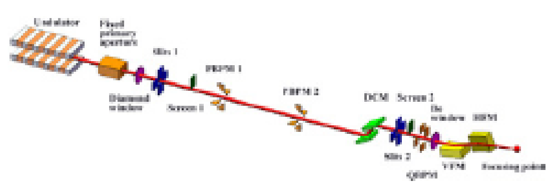
軟物質小角度散射學光束線
(Soft matter small angle scattering)



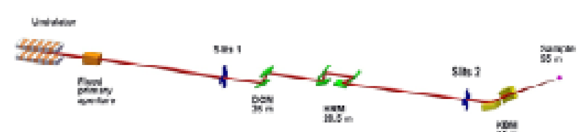
次微米繞射光束線
(Sub- μ x-ray diffraction)



奈米探針光束線
(Nano-probe x-ray diffraction)



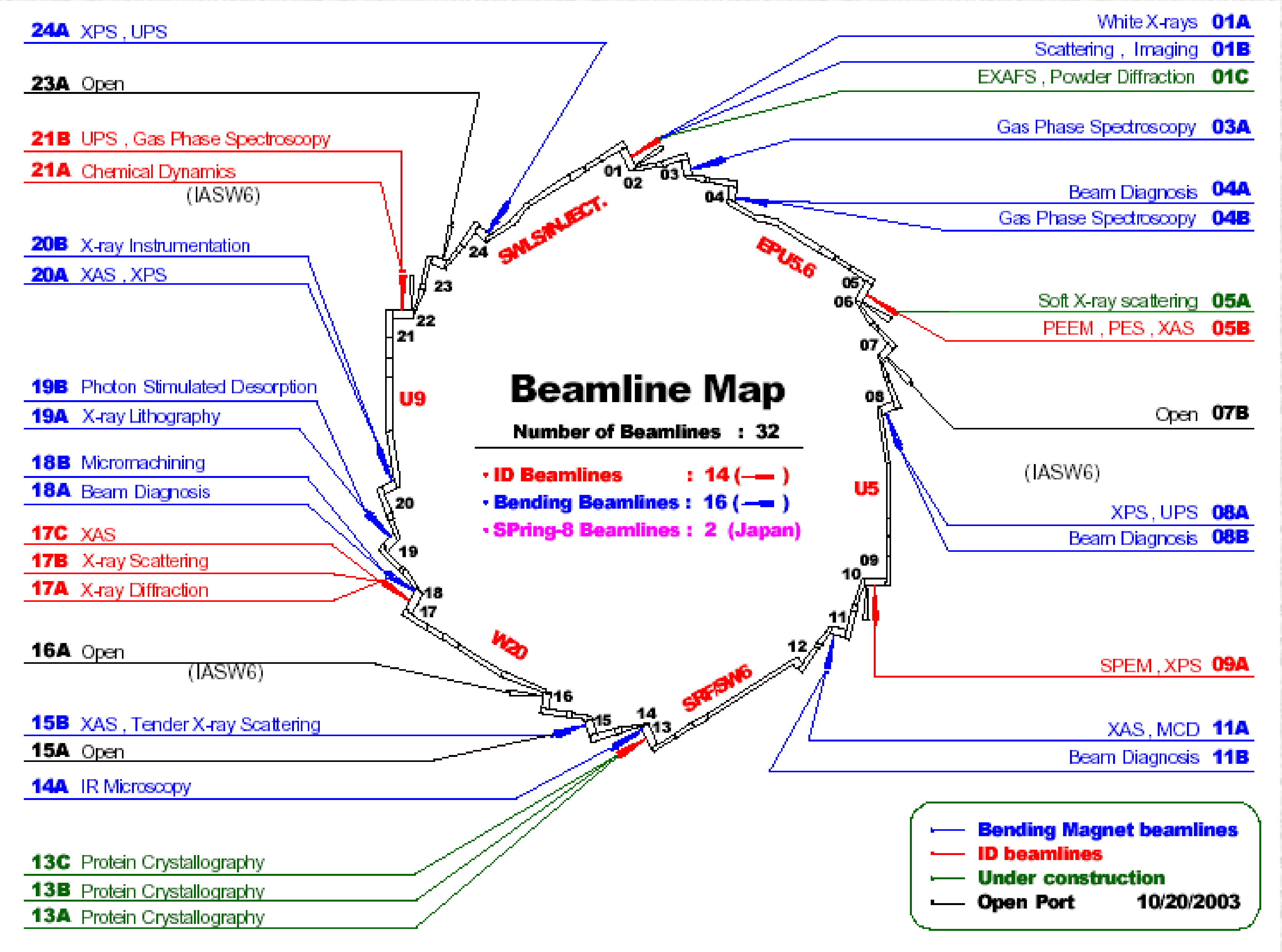
多用途同調性散射光束線
(Multi-purpose coherence x-ray scattering)



謝謝聆聽 ！！

Thank you for your attention !!

NSRRC Beamline



Energy scans