



## **Synchrotron Radiation**

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- What is synchrotron?
- X-ray and synchrotron radiation
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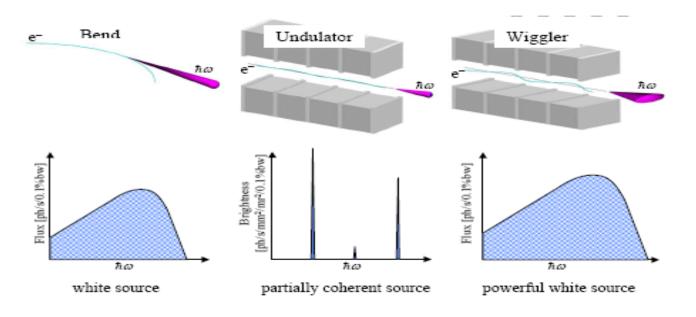
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## What is synchrotron?



## What is synchrotron?

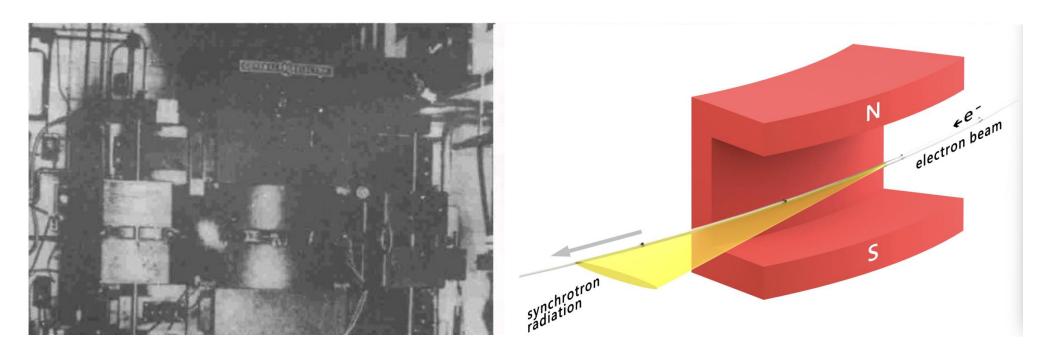
- Synchrotron radiation is the electromagnetic waves (light) radiated along the tangential direction when charged particles at a speed close to that of light change their direction of motion;
- Devices (radiation sources) used to change the direction of movement of charged particles can be bending magnets, undulator and wiggler.





## History of synchrotron radiation

In April 1947, F.R. Elder team observed the electromagnetic radiation from electrons for the first time at the 70MeV electron synchrotron at General Electric Laboratories in the United States, hence the name synchrotron radiation.



1950s, after a series of explorations, people discovered that SR is a very excellent light source.

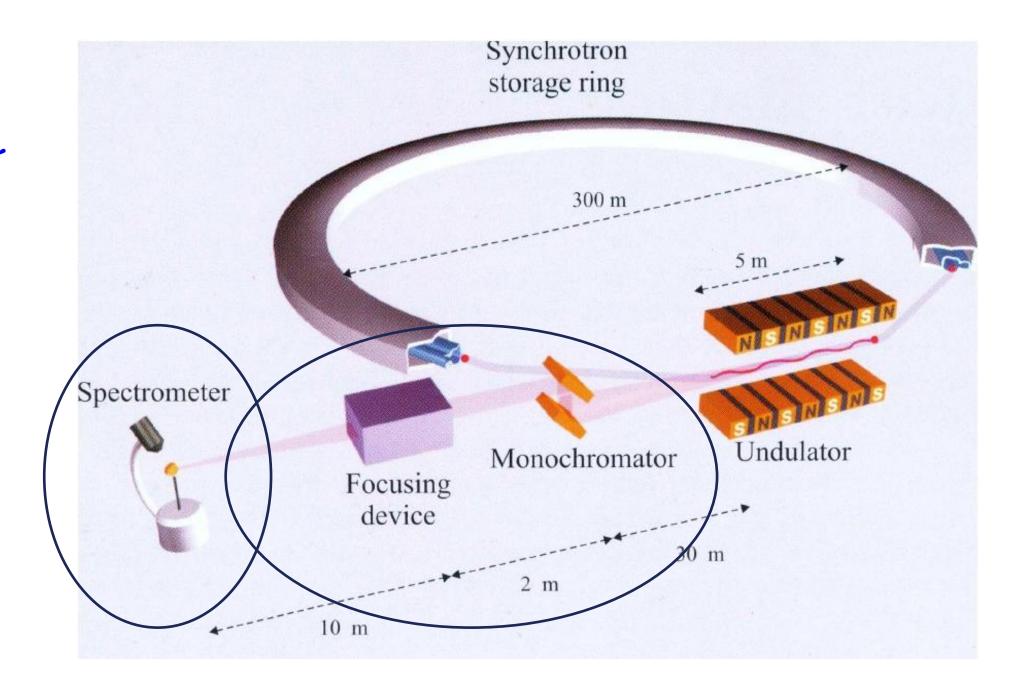
Early 1960s, the application of synchrotron radiation began.

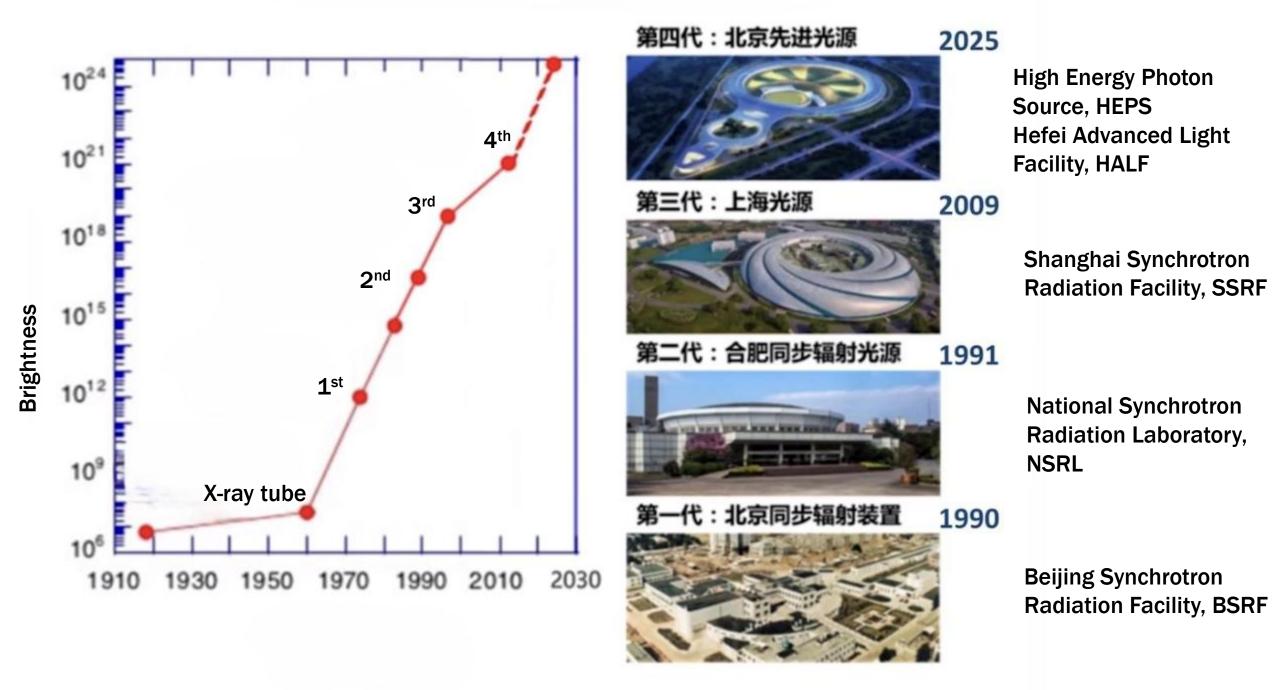
1965, first storage ring built in Frascati.

1970s, the modern stage of synchrotron radiation application began.

# The major parts

- Storage ring with radiation sources
- **♦** Beamline
- **♦** End station

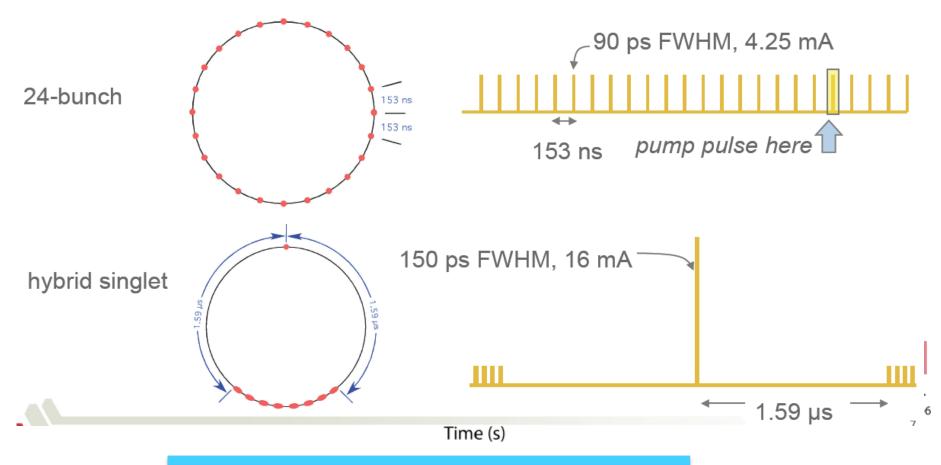




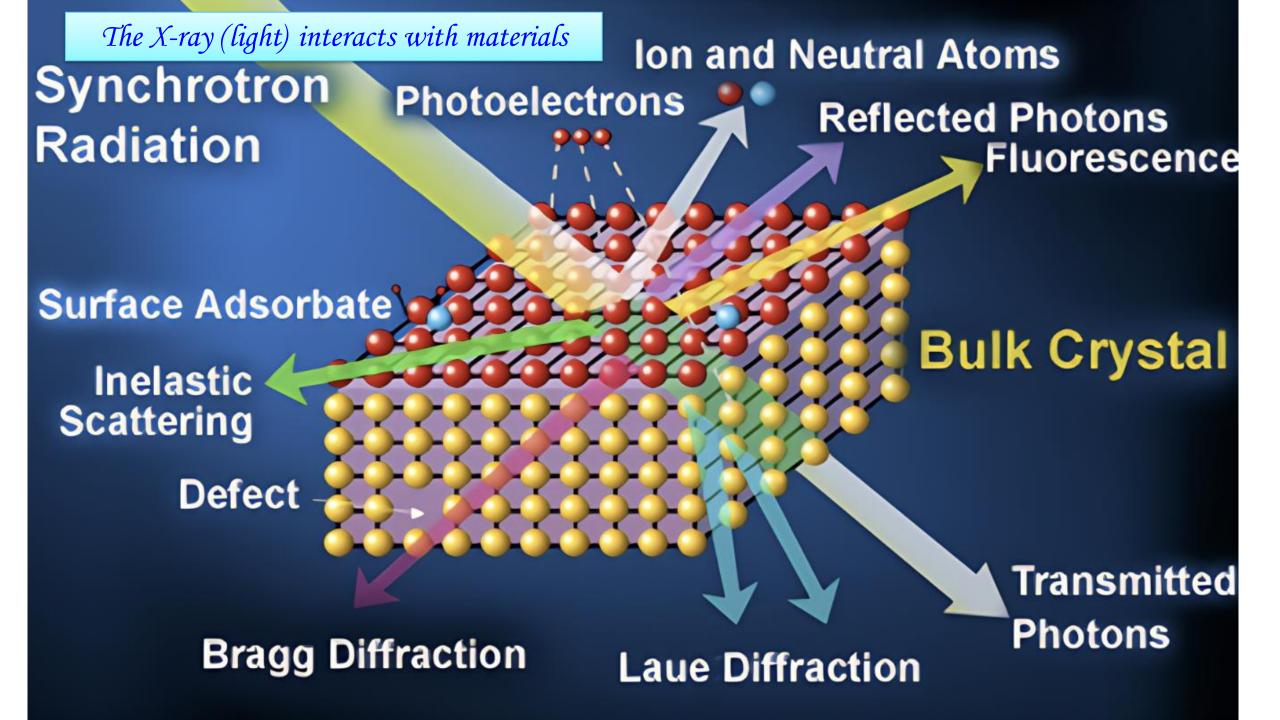
#### The spectrum of synchrotron radiation covers a wide range from infrared to hard X-rays To detect the structure of matter at a certain scale, light with a wavelength that matches it is needed. To detect physical phenomena of a certain energy, we need light with $\lambda = 100 - 0.01 \mathring{A}$ **Nucleus** energy that matches it. LOSS INTENSITY 10<sup>-9</sup> 10<sup>-10</sup> 10-14 10-12 Co1---Surf. Plasmons, (1 nm) (1 Å) (m) Plasm. Surface Core Electronic Å/1.24keV Phonons Level Intersend wavelength Transitions Transmors Soft K-rays Hard X-rays **Gamma Rays** Photon energy 1000 0.01 0.1 100 10 105 106 107 103 (eV) $\varepsilon = 0.124 - 1240 \text{keV}$ So LOSS ENERGY (eV) =124eV-1240keV lioactive Radio **Microwave Light Bulbs** Tube Synchrotron Light Source

## Time structure of synchrotron radiation

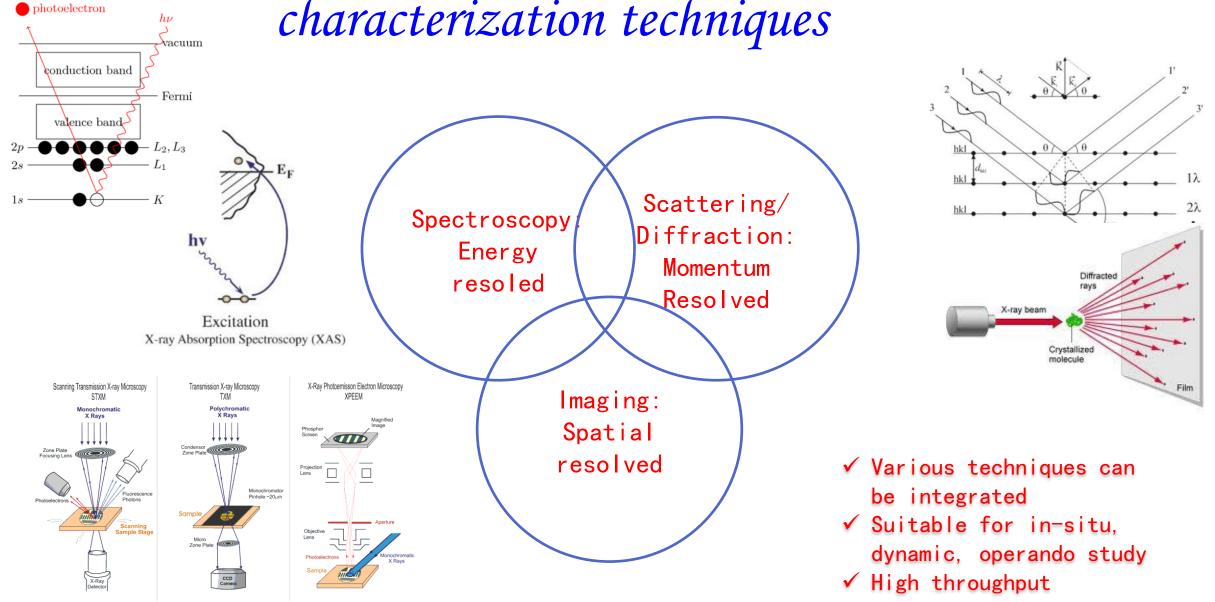
To detect physical processes on a certain time scale, we need light with a temporal structure that matches it.



FEL or slice technology can achieve fs resolution



## Classification of synchrotron-based characterization techniques



### World wide Synchrotron Facilities



	, prop
Arrite Ocean	Aretic Ocean
	MODILE STATES
	Pal William
PETRA-III MAX-II MAX-IV	CLS
Diamond Didoot,UK-	Saskatoon,SK,Canada  Agreement Creedand
SOLEIL Saclay,France Solaris Krakow,Poland Krakow,Poland	APS Argonne, IL, USA
SLS ANKA CANDLE SPRIng	
ESRF Propul ELETTRA STATE SSRF NewSUB	ARU Berkeley,CA,USA NSLS-II
ALBA SESAME Pattern SESAME Pattern SAGA-L	S Stanford, CA, USA
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Synchrotro  Sing ageneration synchrotron under construction 正在世代哲学で同步編集大線  Proposed new synchrotron	Pacific Control of the Control of th
- 日对建设的同步辐射光端 48	Campinas,Brazili

	Faciality	Electro Energy (GeV)	
	ASTRID 2	0.54	
	SOLARIS	1.5	
	MAX-IV	1.5	
S	NSRL (	0.8	
3	BESSY-II	1.7	
	ALS	1.9	
	ELETTRA 2	2/2.4	
	SSRF	3.5	
	TPS	3	
	PLS-II	3	
	SLS	2.4	
	SOLEIL	2.75	
T	CLS	2.9	
	ALBA	3	
	DIAMOND	3	
	MAX-IV	3	
	NSLS-II	3	
	AS	3	
	ESRF	6	
н	PETRA-III	6	
	APS	7	
	SPring-8	8	

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## X-ray and synchrotron radiation



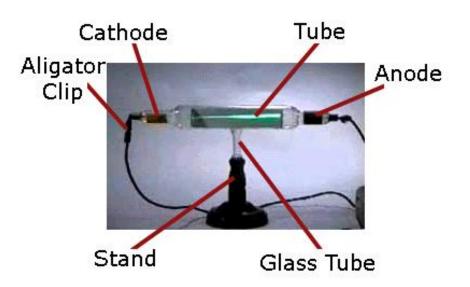
## The discovery of X-ray

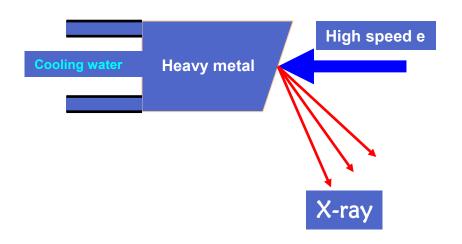
At the end of 1895,
German scientist
Wilhelm Conrad
Röntgen discovered
a mysterious
radiation- X-ray while studying
cathode ray tubes.

- >cathode ray 1858
- > Electron 1897
- >X-ray 1895
- ≻ Radioactivity (α、β、γ) 1896

Electromagnetic technology: high voltage electricity Vacuum technology: obtaining vacuum







## What is X-ray: its nature

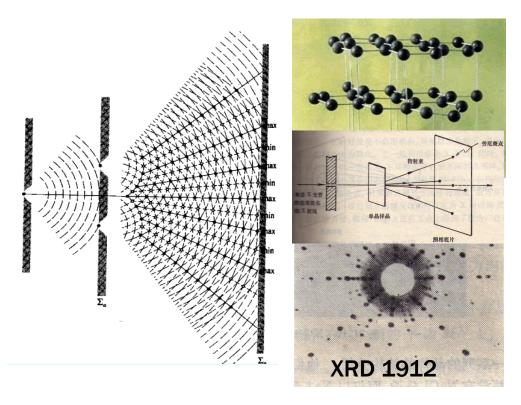
#### ✓ Wave:

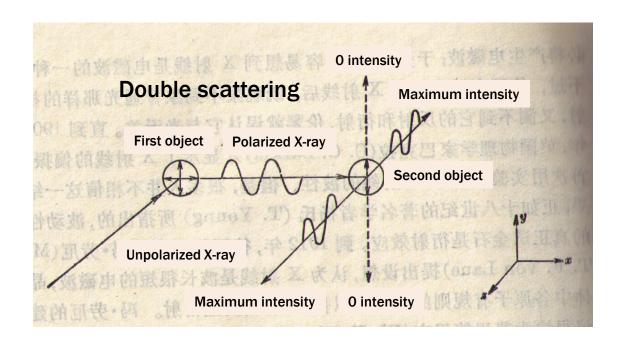
transverse wave not Longitudinal wave: double scattering experiment

✓ particle:

Photoelectric effect: energy quantization

Compton scattering: energy and momentum quantization

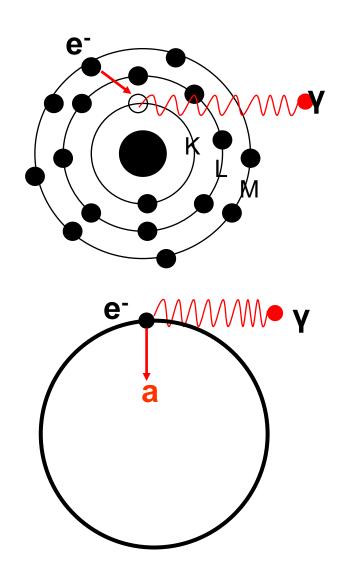




## Generation of X-ray

The electrons in the inner shell of an atom are excited to form holes, and the electrons at the higher energy level jump to the energy level with holes, emitting high energy photons (X-ray);

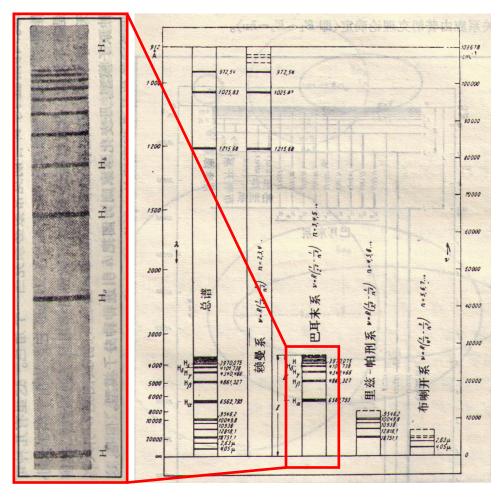
 Radiation produced by accelerated charged particles (electrons).



## Atomic inner shell electron transition

## Atomic photoemission

atomic spectrum



Hydrogen atomic spectrum

#### Balmer's Law:

$$v = \frac{1}{\lambda} = \frac{4}{B} \left( \frac{1}{2^2} - \frac{1}{n^2} \right)$$

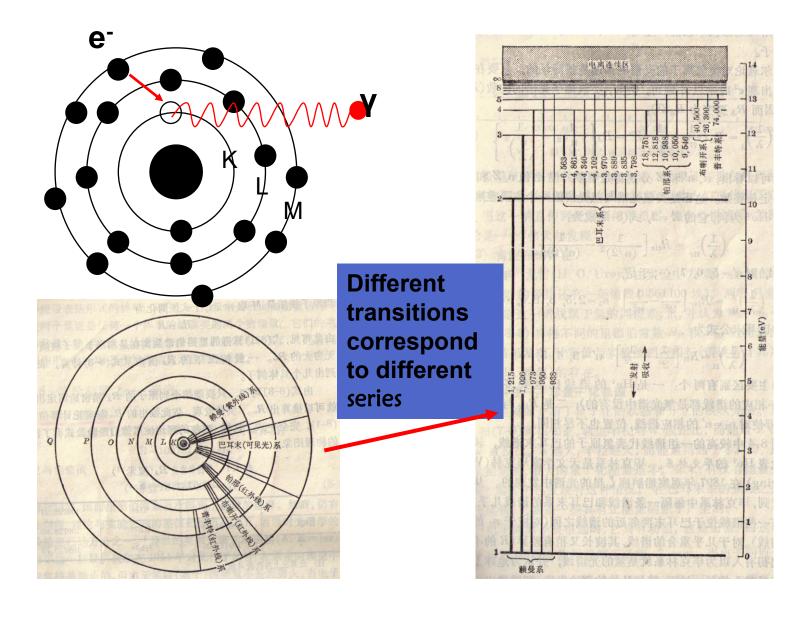
n=3,4,5...
Balmer series

#### Rydberg equation:

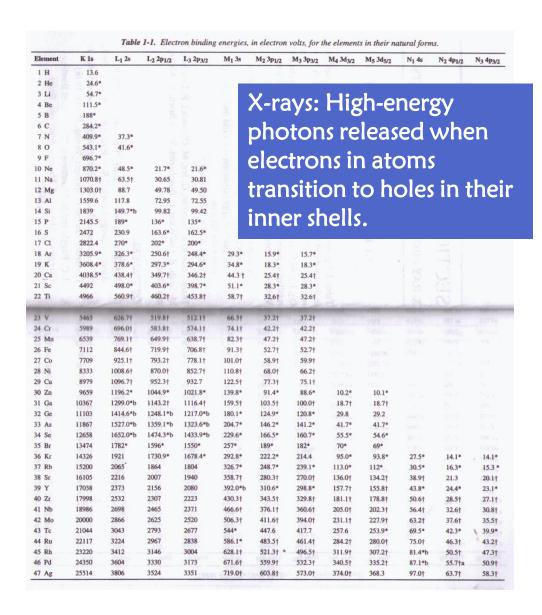
$$v = \frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

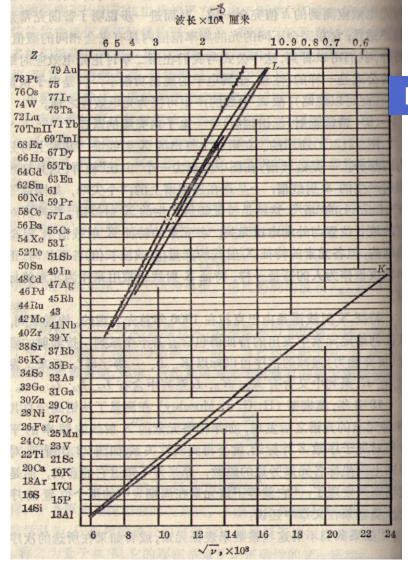
 $n_1=1,2,3...$ Lyman, Balmer, Paschen  $n_2=n_1+1,n_1+2,...$ 

### Electron transitions within an atom



## Electron transitions to the inner shells of an atom

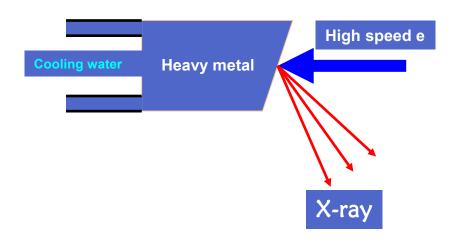


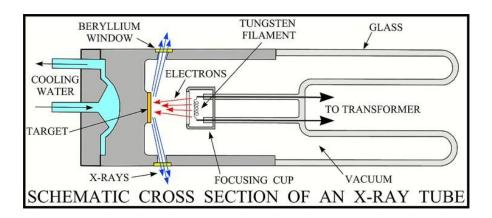


#### Moseley's law

 $\sqrt{v}$  = a(Z - b), where 'v' is the frequency of the emitted X-ray, 'Z' is the atomic number, 'a' is a constant, and 'b' is a screening constant

## *X-ray tube*







## X-ray characteristics generated by X-ray tubes: continuous spectrum

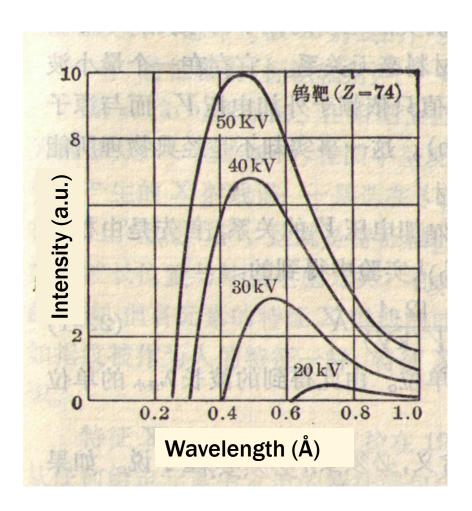
In bremsstrahlung, the energy of the X-ray photon is equal to the energy lost by the electron:

$$T = eV = hv_{\text{max}} = \frac{hc}{\lambda_{\text{min}}}$$

Due to the different collision parameters, the energy loss by electrons in different collision processes is different, which is statistically continuous, so the photon energy spectrum of bremsstrahlung is also continuous.

The maximum energy of the photon (shortest wavelength) corresponds to the maximum energy of the electron:

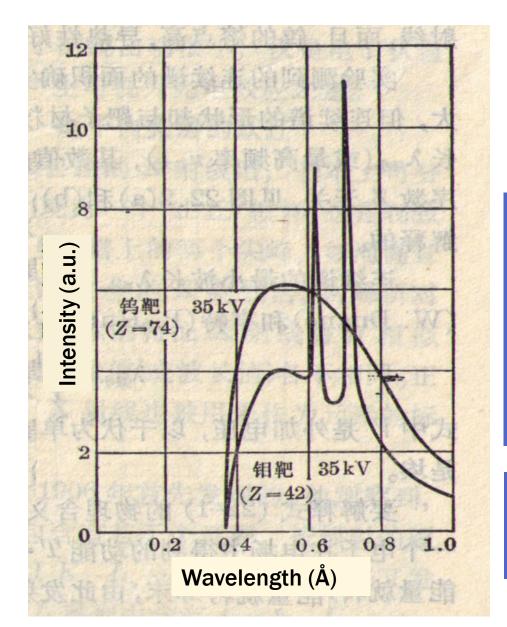
$$\lambda_{\min} = \frac{hc}{eV} = \frac{12.4}{V(kV)} \stackrel{\circ}{A}$$



Wavelength with maximum intensity:  $\lambda_m \approx \frac{3}{2} \lambda_{\min}$ 

$$\lambda_m \approx \frac{3}{2} \lambda_{\min}$$

## X-ray characteristics produced by X-ray tubes - discrete spectra



#### Moseley's Law

$$\nu \propto Z^2$$

$$\nu_{K_{\alpha}} = 0.248 \times 10^{16} (Z - b)^2 \qquad b \approx 2$$

*h*≈1

- 1) For X-ray tubes with the same high voltage and different target anodes, the short wavelength limit is the same;
- 2) The X-ray intensity produced by high-Z target anodes is higher than that produced by low-Z target anodes;
- 3) For the same X-ray tube, as the voltage increases, discrete spectra appear on the continuous spectrum.

X-ray fluorescence spectroscopy: The atomic number Z can be obtained from X-rays, which pioneered the X-ray analysis method.

*X-ray notation* 

## X-ray and spectroscopic notation in j-j coupling

Quar	Quantum numbers				
n	l	j	X-ray suffix	X-ray level	Spectroscopic level
1	0	1/2	1	K.	1s <sub>1/2</sub>
2	0	1 2	1	L,	2s <sub>1/2</sub>
2	1	1 2	2	L,	2p <sub>1/2</sub>
2	1	3	3	L,	2p <sub>3/2</sub>
3	0	<u>1</u>	1	M,	3s <sub>1/2</sub>
3	1	1 7	2	м,	$3p_{1/2}$
3	i	3	3	M <sub>3</sub>	$3p_{3/2}$
3	2	<u>3</u>	4	M.	3d <sub>3/2</sub>
3	2	<u>\$</u>	5	Ms	3d <sub>5/2</sub>
	etc.	•	etc.	etc.	etc.

## X-ray elemental spectrum

 $2p3/2 \rightarrow 1s$  and  $2p1/2 \rightarrow 1s$ Kα1,2 (inseparable) (eV) FWHM (eV) hν Mg 1253.6 0.7 A1 1486.6 0.85 Ionized Mg or Al produces Kα3,4 Higher photon energy than  $K\alpha 1,2$  $\sim 9-10 \text{ eV}$  $3p \rightarrow 1s$ Κβ

#### X-ray lines

	The state of the s	
Line	Energy, eV	Width, eV
ΥΜζ	132.3	0.47
Zr MC	151.4	0.77
NEME	171.4	1.21
ΜοΜζ	192.3	1.53
Ti La	395.3	3.0
Cr La	572.8	3.0
Ni La	851.5	2.5
Cu La	929.7	3.8
Mg Kz	1253.6	0.7
Al Kα	1486.6	0.85
Si Ka	1739.5	1.0
ΥLα	1922.6	1.5
Zr La	2042.4	1.7
Ti Κα	4510.0	2.0
Cr Ka	5417.0	2.1
Cu Ka	8048.0	2.6

X-ray characteristic spectral lines of different elements

## Radiation produced by accelerated electrons

## Radiation produced by accelerated electrons

#### I. The electric field of a moving charge

$$E(r_p,t) = \frac{-e}{4\pi\varepsilon_0} \left[ \frac{(n-\beta)(1-\beta^2)}{r^2(1-n\cdot\beta)^3} + \frac{n\times(n-\beta)\times\dot{\beta}}{cr(1-n\cdot\beta)^3} \right]$$

#### II. Energy flux density of the radiation field

$$S(r_{p},t) = \frac{1}{\mu_{0}c} \left(\frac{e}{4\pi\varepsilon_{0}}\right)^{2} \frac{n}{c^{2}r^{2}} \frac{\left\{n \times \left[(n-\beta) \times \dot{\beta}\right]\right\}^{2}}{(1-n\cdot\beta)^{6}}$$

$$P = \frac{1}{\mu_{0}c^{3}} \left(\frac{e}{4\pi\varepsilon_{0}}\right)^{2} \int \frac{\left\{n \times \left[(n-\beta) \times \dot{\beta}\right]\right\}^{2}}{(1-n\cdot\beta)^{5}} d\Omega$$

#### III. Radiated power distribution

$$E(r_{p},t) = \frac{-e}{4\pi\varepsilon_{0}} \left[ \frac{(n-\beta)(1-\beta^{2})}{r^{2}(1-n\cdot\beta)^{3}} + \frac{n\times(n-\beta)\times\dot{\beta}}{cr(1-n\cdot\beta)^{3}} \right] \qquad \frac{dP}{d\Omega} = \frac{d^{2}W}{dtd\Omega} = r^{2}S(r_{p},t)\cdot n$$

$$= \frac{1}{\mu_{0}c^{3}} \left( \frac{e}{4\pi\varepsilon_{0}} \right)^{2} \frac{\left\{ n\times\left[(n-\beta)\times\dot{\beta}\right]^{2}\right\}}{(1-n\cdot\beta)^{5}}$$

#### IV.total radiated power

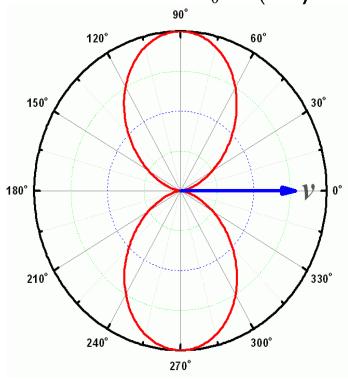
$$P = \frac{1}{\mu_0 c^3} \left( \frac{e}{4\pi\varepsilon_0} \right)^2 \int \frac{\left\{ n \times \left[ (n - \beta) \times \dot{\beta} \right] \right\}^2}{\left( 1 - n \cdot \beta \right)^5} d\Omega$$

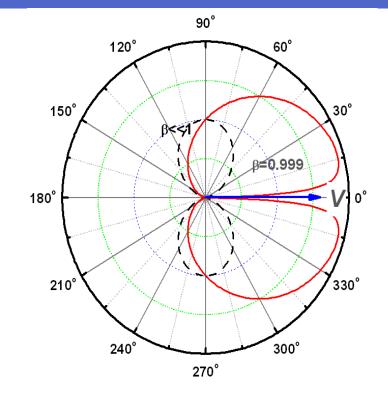
## Acceleration is in the same direction as velocity (opposite direction)

Linear motion: acceleration and velocity are in the same direction (opposite)

$$\frac{dP}{d\Omega} = \frac{e^2 v^2}{16\pi\varepsilon_0 c^3} \frac{\sin^2 \theta}{\left(1 - \beta \cos \theta\right)^5}$$

Radiated power is proportional to the square of acceleration





non-relativistic:  $\beta <<1$ 

relativistic:  $\beta \rightarrow 1$ 

## Radiation intensity of electrons moving in a straight line

#### **Electron Linear Accelerator**

#### Radiation intensity and energy gain ratio:

$$\frac{P}{dE/dt} \propto \frac{1}{\beta} \frac{\frac{dE}{dx}}{mc^2/\frac{e^2}{mc^2}}$$

Electron Linear Accelerator,

$$dE/_{dx} \approx 10 \ keV/m = 10^{-17} \ MeV/_{fm}$$

Radiation loss can be basically ignored

#### Bremsstrahlung

$$E_K = E_0 - \frac{e^2}{x}$$

$$E_K = \mathbf{0} \qquad x_{\min} = \frac{e^2}{E_0}$$

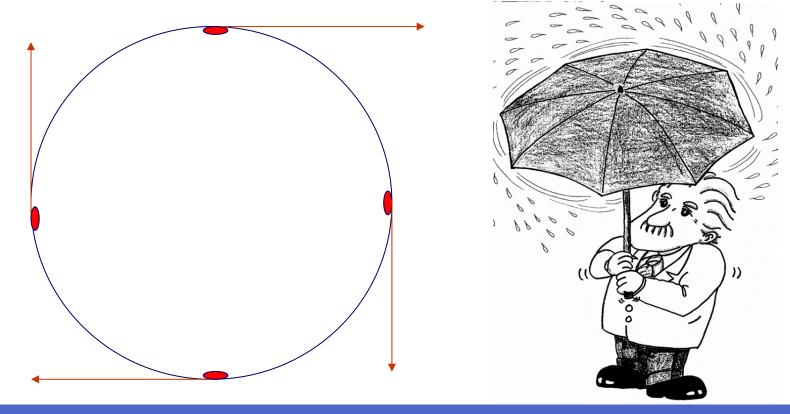
$$\frac{dE_K}{dx} = \frac{e^2}{x^2} \qquad \frac{dE_K}{dx}_{\max} = \frac{E_0^2}{e^2}$$

$$E_0 = 10keV \qquad \frac{dE_K}{dx} - 5 \frac{MeV}{fm_{\max}}$$

Much larger than the radiation power and energy change ratio in the electron linear accelerator

## The direction of acceleration is perpendicular to the direction of velocity: synchrotron radiation

Synchrotron radiation is an electromagnetic wave (light) emitted by charged particles (electrons) moving at close to the speed of light in an ultra-high vacuum environment when they change their direction of motion.



Discovered in 1947 on a synchrotron (70MeV), so it is called "synchrotron radiation"

## Radiation from circular motion of electrons

 $\dot{\beta} \perp \beta$  The angle between the observation direction n and the direction of β : θ

#### Distribution of radiated power:

$$\frac{dP}{d\Omega} = \frac{1}{\mu_0 c^3} \left( \frac{e}{4\pi\varepsilon_0} \right)^2 \frac{\left\{ n \times \left[ (n - \beta) \times \beta \right] \right\}^2}{(1 - n \cdot \beta)^5}$$

$$= \frac{e^2 v}{16\pi^2 \varepsilon_0 c^3} \frac{1}{(1 - \beta \cos \theta)^3} \left[ 1 - \frac{\sin^2 \theta \cos^2 \phi}{\gamma^2 (1 - \beta \cos \theta)^2} \right]$$

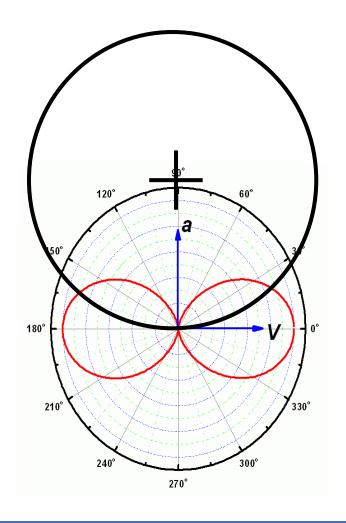
### Radiation from the circular motion of electrons (non-relativistic)

non-relativistic,  $\beta << 1$   $\gamma \approx 1$  radiation power distribution:

$$\frac{dP}{d\Omega} = \frac{e^2 v}{16\pi^2 \varepsilon_0 c^3} \left(1 - \sin^2 \theta \cos^2 \phi\right)$$
$$= \frac{e^2 v}{16\pi^2 \varepsilon_0 c^3} \sin^2 \chi$$

O is the angle between the observation direction and the acceleration direction. In the plane of electron motion, Radiated power distribution:

$$\frac{dP}{d\Omega} = \frac{e^2 v^2}{16\pi^2 \varepsilon_0 c^3} \left(1 - \sin^2 \theta\right)$$



Radiated power is proportional to the square of acceleration.

Non-relativistic Radiation power distribution of circular motion electrons

## Radiation from the circular motion of electrons (relativistic)

relativistic, 
$$\beta \to 1$$
,  $\gamma = \frac{1}{\sqrt{1-\beta^2}}$   $1-\beta \approx \frac{1}{2\gamma^2}$ 

$$\theta \sim 0$$
  $\cos \theta = 1$   $\sin \theta = \theta$ 

In In the plane of the electron orbital, Radiated power distribution:

$$\frac{dP}{d\Omega} = \frac{e^2 v^2 \gamma^6}{2\pi^2 \varepsilon_0 c^3 (1 + \gamma^2 \theta^2)} \left( 1 - \frac{4\gamma^2 \theta^2 \cos^2 \phi}{(1 + \gamma^2 \theta^2)^2} \right)$$

0.4 0.0 +80° 0.6 270°

Radiated power is proportional to the square of acceleration.

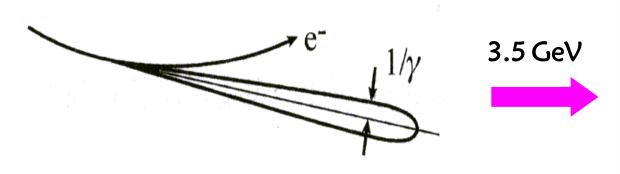
Relativistic Radiation power distribution of circular motion electrons

## Radiation from the circular motion of electrons (relativistic)

The root mean square average of  $\theta$   $\left\langle \theta^{2}\right\rangle ^{\frac{1}{2}}$ 

$$\langle \theta^2 \rangle = \frac{\int \theta^2 \frac{dP}{d\Omega} d\Omega}{\int \frac{dP}{d\Omega} d\Omega} \approx \frac{1}{\gamma^2}$$

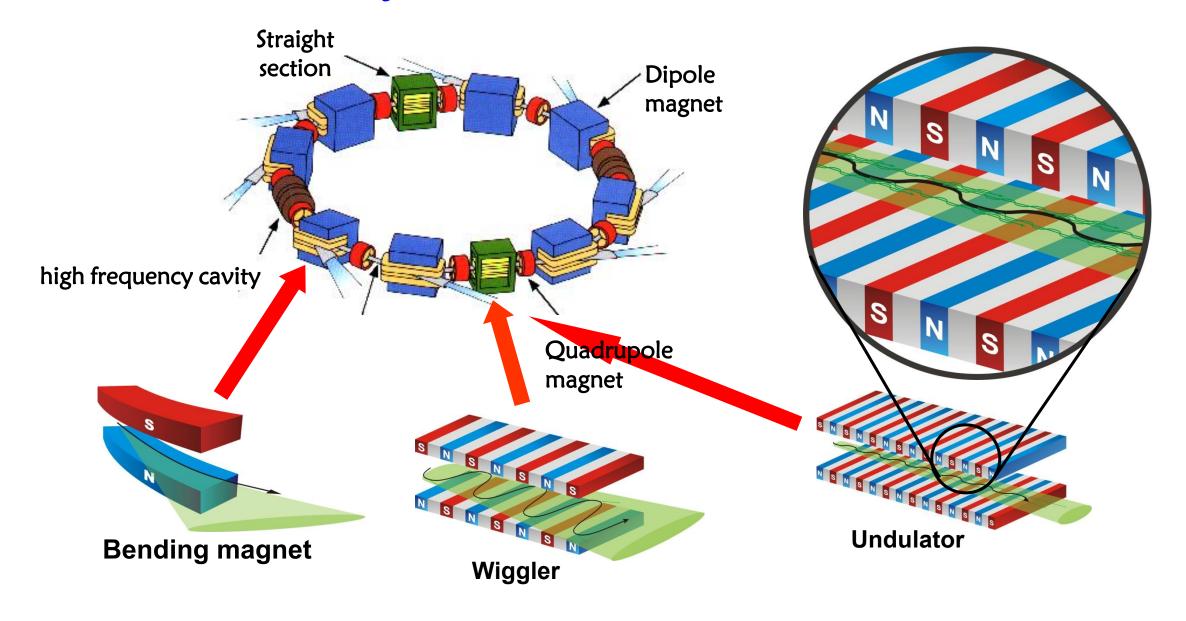
$$\left\langle \theta^{2} \right\rangle = \frac{\int \theta^{2} \frac{dP}{d\Omega} d\Omega}{\int \frac{dP}{d\Omega} d\Omega} \approx \frac{1}{\gamma^{2}} \qquad \left\langle \theta^{2} \right\rangle^{\frac{1}{2}} = \frac{1}{\gamma} = \frac{mc^{2}}{E} = 0.511/E_{e}(GeV)(mrad)$$



0.2 0.0 -0.05 -0.04 -0.03 -0.02 -0.01 0.00 0.01 0.02 0.03 0.04 0.05

Radiation Distribution of Relativistic Electrons in Circular Motion

## Synchrotron radiation sources



## Bending magnet

$$\left\langle \theta^2 \right\rangle^{\frac{1}{2}} = \frac{1}{\gamma} = \frac{mc^2}{E} = 0.511/E_e(GeV)(mrad)$$

#### Radiated power:

$$\frac{dP}{d\Omega} = \frac{e^2 v^2}{16\pi^2 \varepsilon_0 c^3} \frac{1}{\left(1 - \beta \cos \theta\right)^3} \left[ 1 - \frac{\sin^2 \theta \cos^2 \phi}{\gamma^2 \left(1 - \beta \cos \theta\right)^2} \right]$$

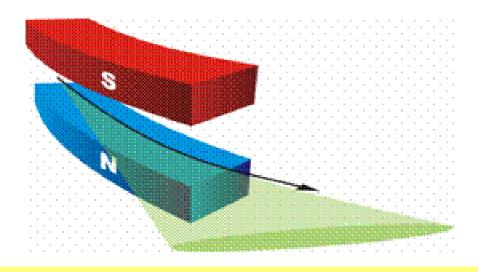
$$P = \int \frac{dP}{d\Omega} d\Omega = \frac{e^2 v^2}{16\pi^2 \varepsilon_0 c^3} \int_0^{\pi/2} \frac{\sin \theta}{(1 - \beta \cos \theta)^3} d\theta \int_0^{2\pi} \left\{ 1 - \frac{\sin^2 \theta \cos^2 \phi}{\gamma^2 (1 - \beta \cos \theta)^2} \right\} d\phi$$
$$= \frac{e^2 v^2}{16\pi \varepsilon_0 c^3} \int_0^{\pi/2} \frac{\sin \theta d\theta}{(1 - \beta \cos \theta)^3} \left\{ 2 - \frac{\sin^2 \theta}{\gamma^2 (1 - \beta \cos \theta)^2} \right\} \approx \frac{e^2 v^2 \gamma^4}{6\pi \varepsilon_0 c^3}$$

## The total energy radiated by an electron in one circle

$$E_r = \frac{e^2 \gamma^4}{3R\varepsilon_0} = 88.5 \frac{E_e^4 (GeV)}{R(m)} (keV)$$

#### The total power for beam current $I_e(A)$

$$P = 88.5 \frac{E^{4}(GeV)I_{e}(A)}{R(m)}(kW) = 26.54B(T)E_{e}^{3}(GeV)I_{e}(A)(kW)$$



#### SSRF:

Electron energy:  $E_e = 3.5 GeV$ 

BM magnetic field strength: B = 1.27T

Emission angle:  $\langle \theta^2 \rangle^{\frac{1}{2}} = 0.146 mrad = 0.0084^{\circ}$ 

The total energy radiated by an electron in one circle

$$E_r = 1446 keV$$

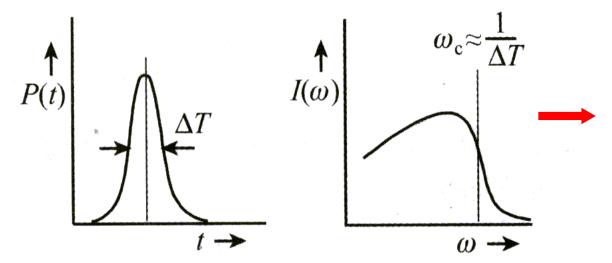
Beam current:  $I_e = 200 mA$ 

Total power: P = 289kW

#### Bending magnet: Energy Spectrum

The time the electron takes to travel within  $\left\langle \theta^{2}\right\rangle ^{\frac{1}{2}}$ 

$$\Delta T = (1 - n \bullet \beta) \frac{2R}{\gamma c \beta} \approx \frac{R}{c} \frac{1}{\gamma^3}$$



The energy spectrum can be obtained by using Fourier transform

#### **SSRF**

$$E_e = 3.5 GeV$$
  
 $R = 9.186m$   
 $\Delta T = 9.63 \times 10^{-20} s$ 

$$I_{(\varpi)} \propto \frac{\sin^2\left(\Delta T \varpi/2\right)}{\left(\varpi/2\right)^2}$$

(Paricle Accelerator Physics Helmut Wiedemann)

### Bending magnet: Energy Spectrum

$$P_{(\varpi)} = \frac{\sqrt{3}e^2\gamma}{8\pi^2\varepsilon_0 R} \frac{\varpi}{\varpi_c} \int_{\varpi/\varpi}^{\infty} K_{\frac{5}{3}}(\eta) d\eta$$
 Bessel function

Critical frequency: 
$$\varpi_c = \frac{3\gamma^3 c}{2R}$$

Critical frequency:  $\varpi_c = \frac{3\gamma^3 c}{2R}$  Critical frequency, or characteristic frequency, is the frequency at which the energy (power) is the same on both sides.

Critical energy: 
$$\varepsilon_c = \frac{h}{2\pi} \varpi_c = 2.22 \frac{E^3 (GeV)}{R(m)} (keV) = 0.665 B(T) E_e^2 (GeV)$$

An electron beam with energy  $E_e(GeV)$  and flux  $I_e(mA)$  radiates photons per unit time and per unit energy width per unit solid angle.

$$\frac{dN_r}{dtd\psi(\Delta \varpi/\varpi)} = 2.457 \times 10^7 E_e(GeV)I_e(mA)G_1(\varpi/\varpi_c)(photons/s/mrad/0.1\%BW)$$

G function: 
$$G_1\left(\frac{\varpi}{\varpi_c}\right) = \frac{\varpi}{\varpi_c} \int_{\varpi_c}^{\infty} K_{\frac{5}{3}}(\eta) d\eta$$

## The spectrum of SSRF bending magnet

#### **Electron energy**

$$E_e = 3.5 GeV$$

#### **Magnetic field strength**

$$B = 1.27T$$

#### **Emission angle**

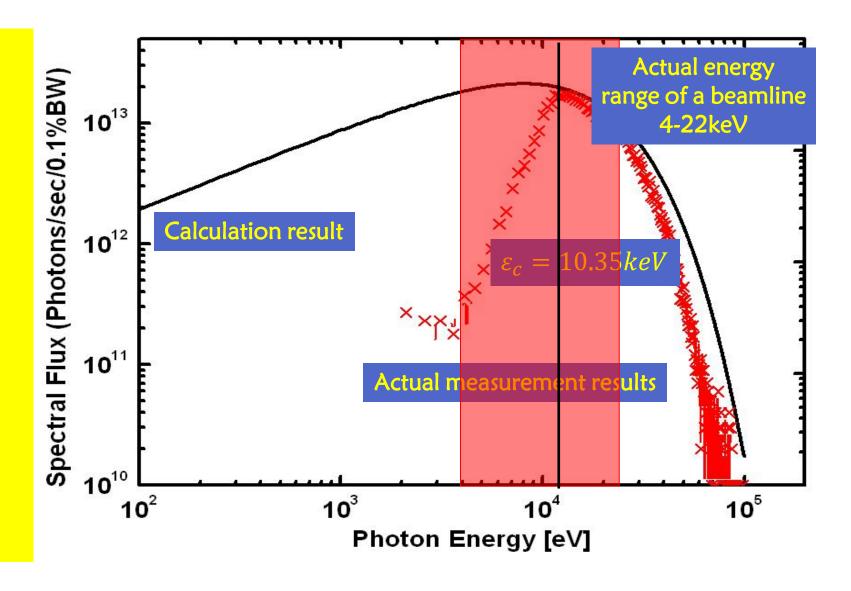
$$\langle \theta^2 \rangle^{1/2} = 0.146 mrad = 0.0084^{\circ}$$

The total radiation energy of an electron after one circle:

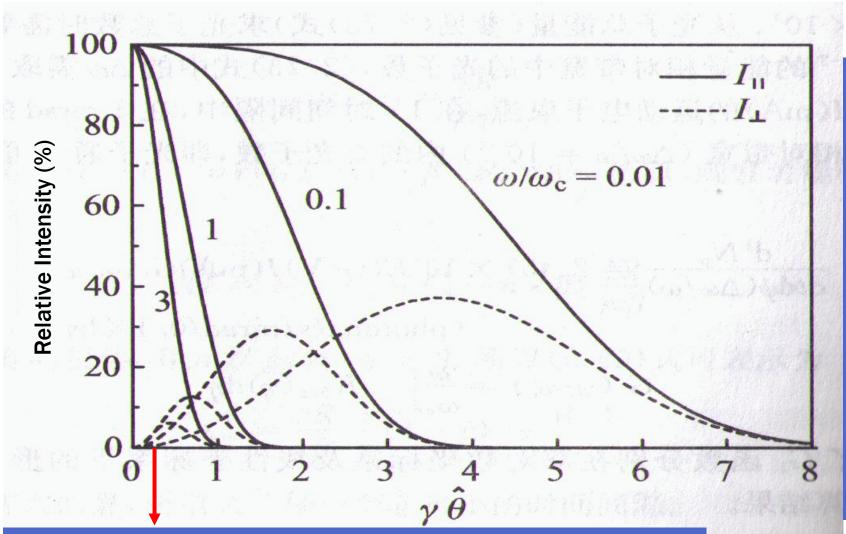
$$E_r = 1446 keV$$

$$\varepsilon_c = 10.35 keV$$

$$I_e = 200mA \qquad P = 289kW$$



## X-ray polarization from a bending magnet



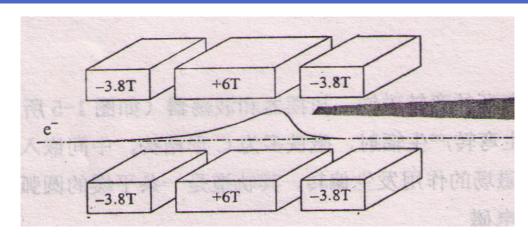
The degree of polarization depends on the photon energy: the higher the energy, the stronger the horizontal component.

The greater the deviation from the electron orbital plane, the stronger the vertical component.
Above this plane, linear polarization to elliptical polarization, to circular polarization.

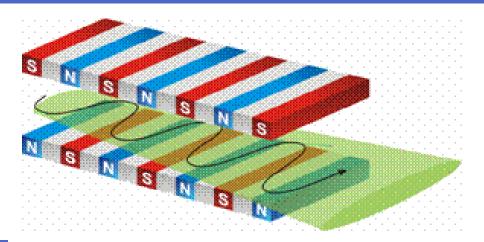
Only when  $\theta = 0$  (in the XZ plane) it is linear polarization.

## Insertion device: Wiggler

Composed of multiple pairs of magnets with opposite directions. The period of the magnets is longer and the period number N is smaller. The electrons do not emit light once like in the bent iron, but change the direction of movement many times and emit light in the same solid angle, but the photons have no correlation with each other (incoherent). The photon energy spectrum, characteristic energy and other parameters of the wiggler are the same as those of the bent iron light source with the same magnetic field strength, but the local magnetic field strength is increased, which can increase the photon energy. The total photon intensity is 2N times that of a single magnet:  $I_W = 2NI_{BM}$ 



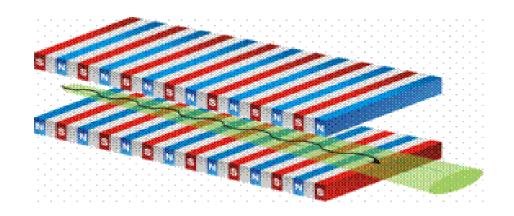
Monopole wiggler (frequency shifter): composed of 3 dipole magnets, which enhance the local magnetic field and increase the photon energy, while the electron orbit remains unchanged at the entrance and exit.

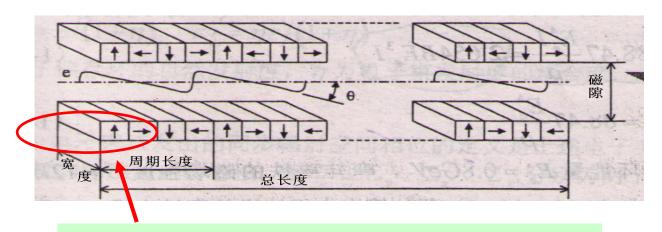


Multipolar Wiggle: consists of N magnetic field pairs with opposite polarities. (Equivalent to 2N bent iron light sources)

#### Insertion device: Undulator

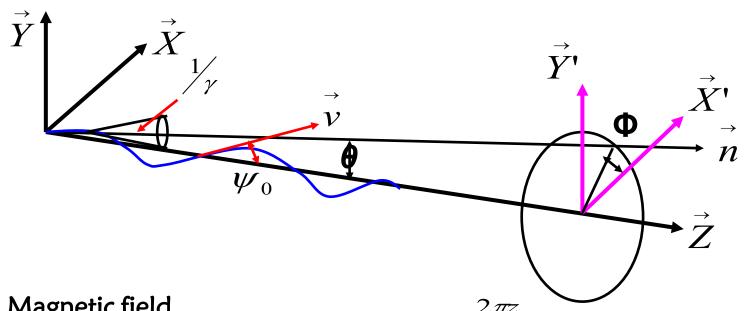
Undulator: composed of multiple magnet pairs. Its magnetic field strength is weak, but the period is short and the number of periods is large. Electrons move in a very small sine wave in a magnet group with opposite polarity. The radiation generated in each period is coherent. In the final emitted light, the wavelength of light that meets the coherent enhancement condition will be enhanced, and its brightness is N<sup>2</sup> times the brightness of a single-period magnet light source. The wavelength of light that does not meet the enhancement condition is weakened, so its spectrum is discontinuous.





The polarity of the magnet is not simply NS or SN.

## The spectrum of X-ray from a undulator



The magnetic field strength B<sub>0</sub> is weak, the period length λu is short, the electrons move in a sinusoidal motion with a smaller amplitude.

Magnetic field strength in Y direction:

$$B_{y} = B_{0} \sin \frac{2\pi z}{\lambda_{u}}$$

Electron motion:

$$x(z) = \frac{\lambda_u}{2\pi} \frac{K}{\gamma} \cos(\frac{2\pi}{\lambda_u})$$

Deflection factor:

$$K = \frac{eB_0 \lambda_u}{2\pi mc} = 0.934 \lambda_u (cm) B_0 (T)$$

$$\gamma = \frac{E_e}{mc^2} = 1957 E_e (GeV)$$





## The spectrum of X-ray from a undulator

The equation of motion of the electron in the undulator is sinusoidal, and the energy spectrum obtained from the Fourier transform is a quasi-monochromatic spectrum. The wavelength that satisfies coherent enhancement is:

$$\lambda_n = \frac{\lambda_u}{2n\gamma^2} \left[ 1 + \frac{K^2}{2} + (\gamma \theta)^2 \right]$$
 When K<<1,  $\lambda_1 = \frac{\lambda_u}{2\gamma^2}$  quasi-monochromatic, coherent, parallel beam

$$\lambda_1 = \frac{\lambda_u}{2\gamma^2}$$

In the forward direction, there are only odd harmonics, n=1,3,5,7...

Along z axis,  $\theta = \psi = 0$ , When n=1, that is, the fundamental wave, the fundamental wave energy:

$$\varepsilon_{1} = \frac{0.95E_{e}^{2}(GeV)}{(1+K^{2}/2)\lambda_{u}(cm)}(keV)$$

An electron beam with  $E_e(GeV)$  energy and  $I_e(mA)$  flux radiates photons per unit time and per unit energy width per unit solid angle.:

$$\frac{dN_{\gamma}}{dtd\psi(\Delta\omega/\omega)}\bigg|_{\theta=0} = 1.744 \times 10^{11} N_u^2 E_e^2 (GeV) I_e(mA) F_n(K) (photons/s/mrad/0.1\%BW)$$

The radiation intensity is proportional to the square of the number of magnetic field periods Nu.

#### The spectrum of X-ray from a undulator

$$F_n(K) = \frac{n^2}{(1 + K^2/2)^2} |E_{nx}|^2$$
 n an odd number

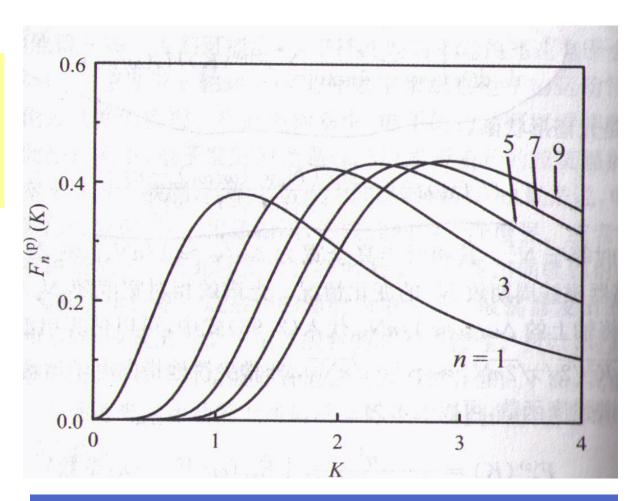
n an even number

$$|E_{nx}| = K |J_{(n+1)/2}(Y_0) - J_{(n-1)/2}(Y_0)|$$

$$Y_0 = \frac{nK^2}{(4+2K^2)}$$

J is Bessel function

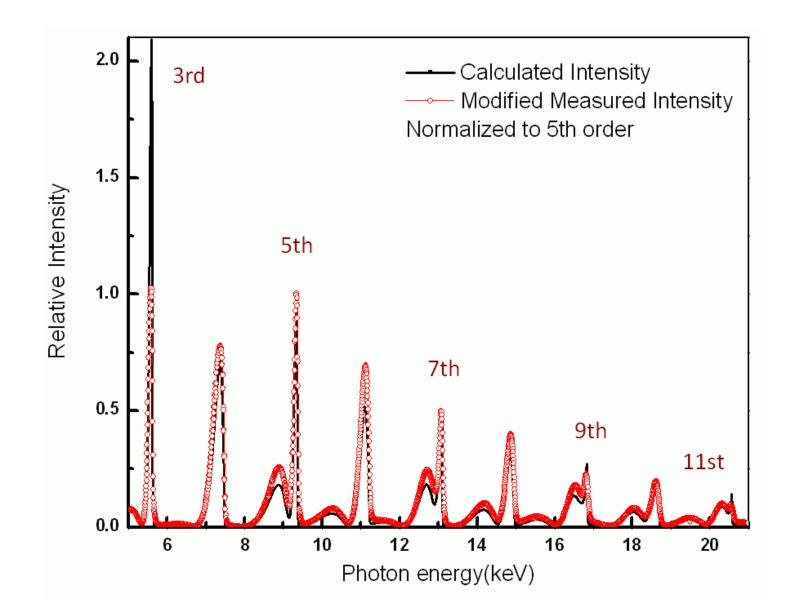
$$K = \frac{eB_0 \lambda_u}{2\pi mc} = 0.934 \lambda_u (cm) B_0 (T)$$



Adjusting K (magnetic field strength B) can change the maximum intensity wavelength

#### Energy spectrum of IVU source at SSRF

IUV25 : B=0.95T@Gap=7 mm T=25 mm Nu=80



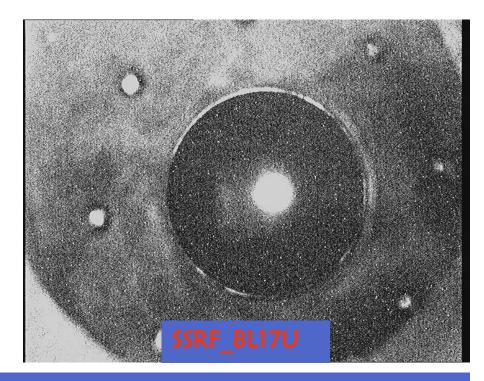
#### Angular distribution of the beam of an undulator source

#### Divergence angle of the undulator beam

$$\theta_{1/2} \approx \frac{\sqrt{1 + \frac{K^2}{2}}}{\gamma^2 \sqrt{2nN_u}} \approx \frac{1}{\gamma} \frac{1}{\sqrt{2nN_u}}$$

Divergence angle of bending magnet source

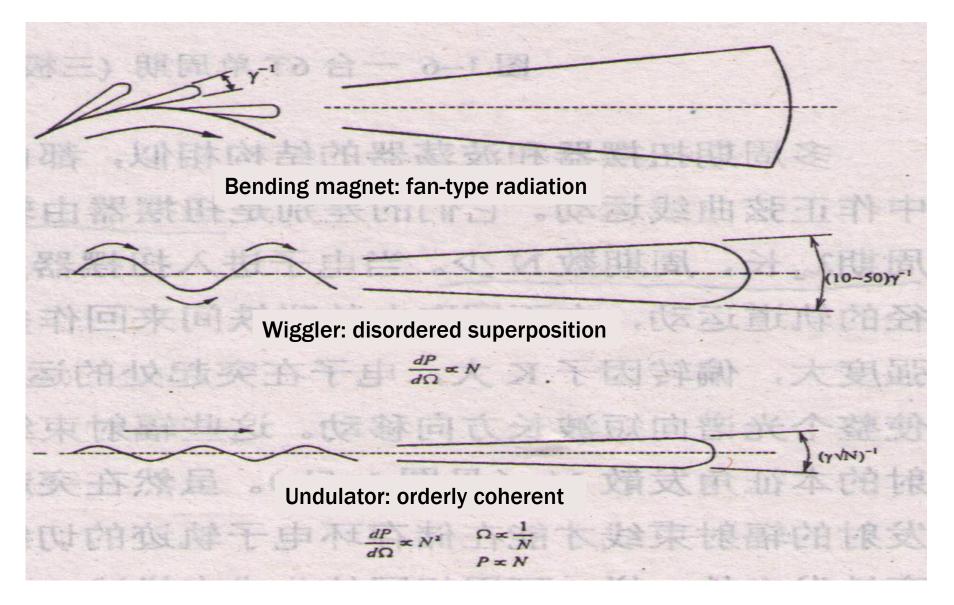
$$\left\langle \theta^{2}\right\rangle ^{1/2}$$



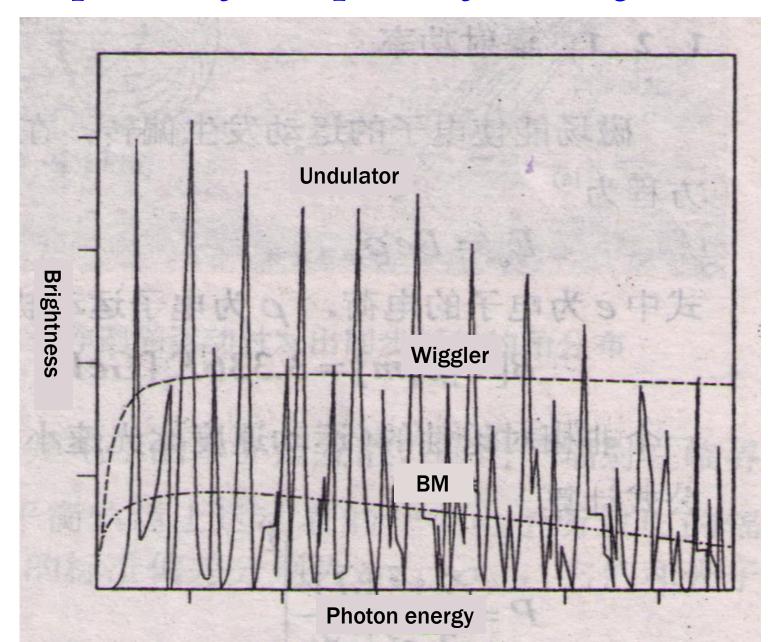
The undulator is a plane undulator, that is, the electrons move in the XZ plane, and the radiation generated is linearly polarized in the XZ plane.

If the magnetic field is a spiral distribution rotating around a certain axis, elliptically polarized radiation can be generated.

## Comparison of the principles of three light sources



# Comparison of the spectra of three light sources



## Advantages of synchrotron light sources

Wide energy spectrum: capable of producing full-band radiation from far infrared to hard X-rays;

Monochromatic: produced by electrons in an ultra-high vacuum environment and further monochromatized by the beamline optics.

High collimated: since the divergence angle of the emitted electron beam can be controlled to be very small, the divergence angle of the emitted light is also very small, with high collimation;

High brightness and high flux: since very high-power radiation is concentrated in a very small spot, synchrotron radiation has very high power (flux) and brightness

High polarization: synchrotron radiation is the emission of electrons in a magnetic field. By controlling the structure of the magnetic field and the extraction position of the light, a beam with good polarization can be obtained.

Stable time structure: since the energy of the electron bunch running in the accelerator is very stable, synchrotron radiation has a stable pulse time structure and can be used for time process research;

Precise predictability: since synchrotron radiation is radiation caused by precise charge movement, its energy spectrum, brightness and other parameters can be accurately calculated based on electron energy, beam current, magnetic field strength and other parameters, and can be used as a standard light source;

Coherence: partial coherence, quasi-coherence.

03

# X-ray interaction with matter

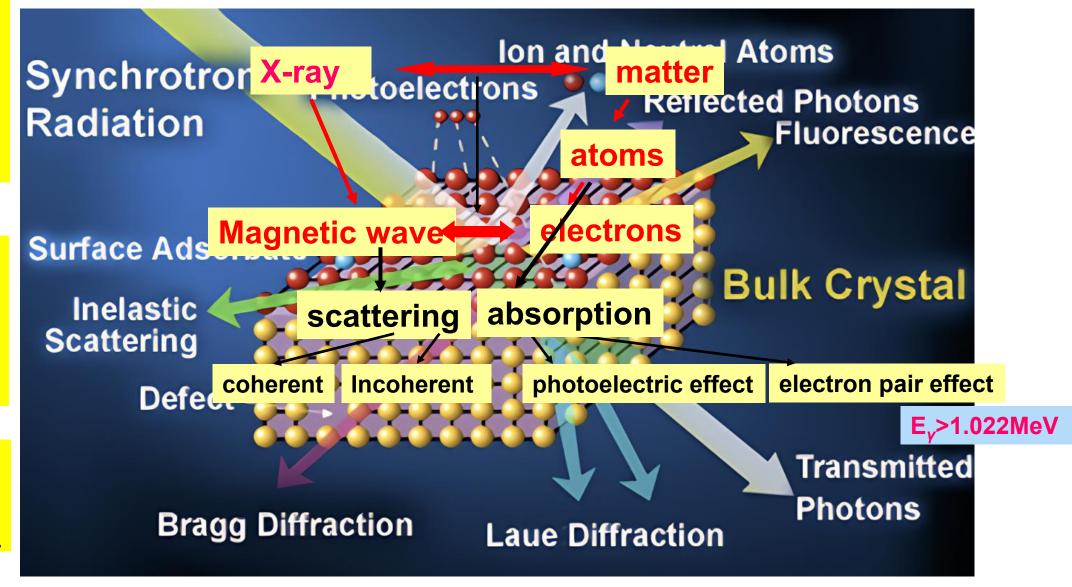


Photoelectric effect produce photoelectrons with a certain kinetic energy, and produces secondary characteristic fluorescence radiation or Auger electrons

Incoherent
scattering: Direction
and frequency
change, the electron
gains a certain
amount of energy
and momentum

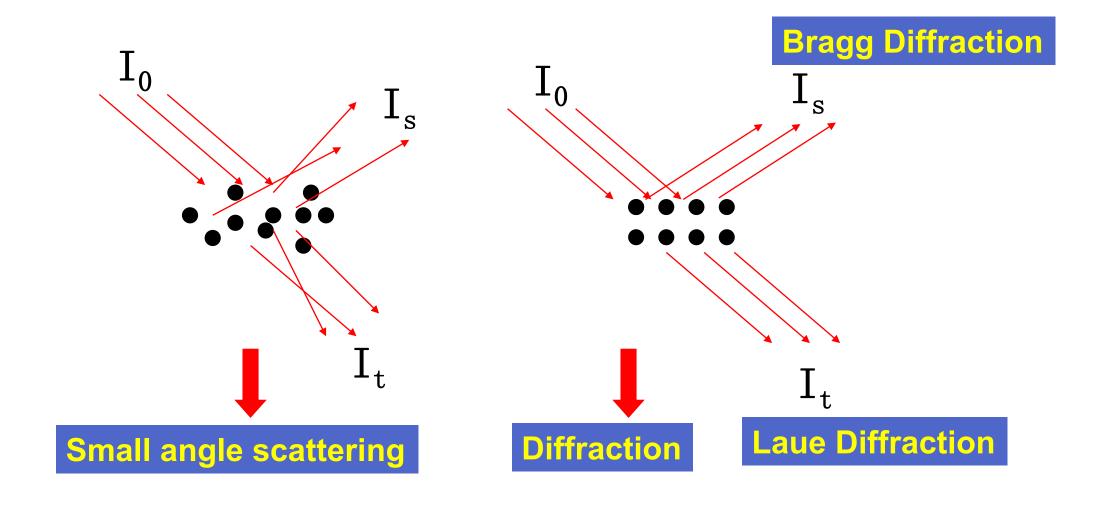
Coherent/classical
/Thomson scattering:
direction may be
changed, the
frequency unchanged.

## *X-ray interaction with matter*



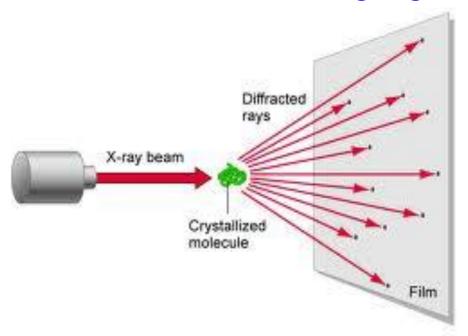
# X-ray Scattering

# Coherent scattering (Thomson scattering)



# X-ray scattering/Diffraction

#### Diffraction: long range order

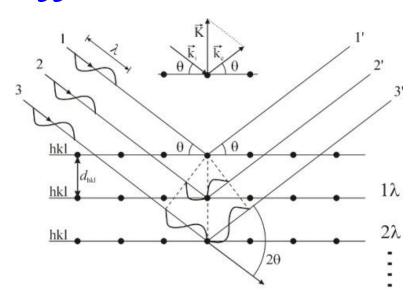


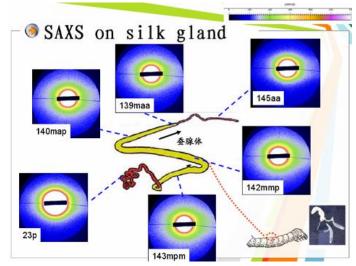
Real space



reciprocal space

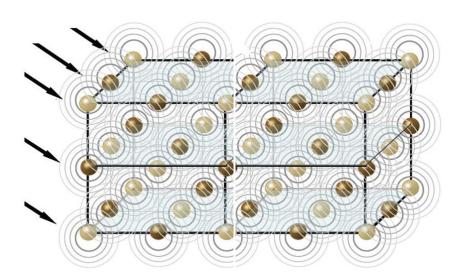
Scattering: average microscopic morphology



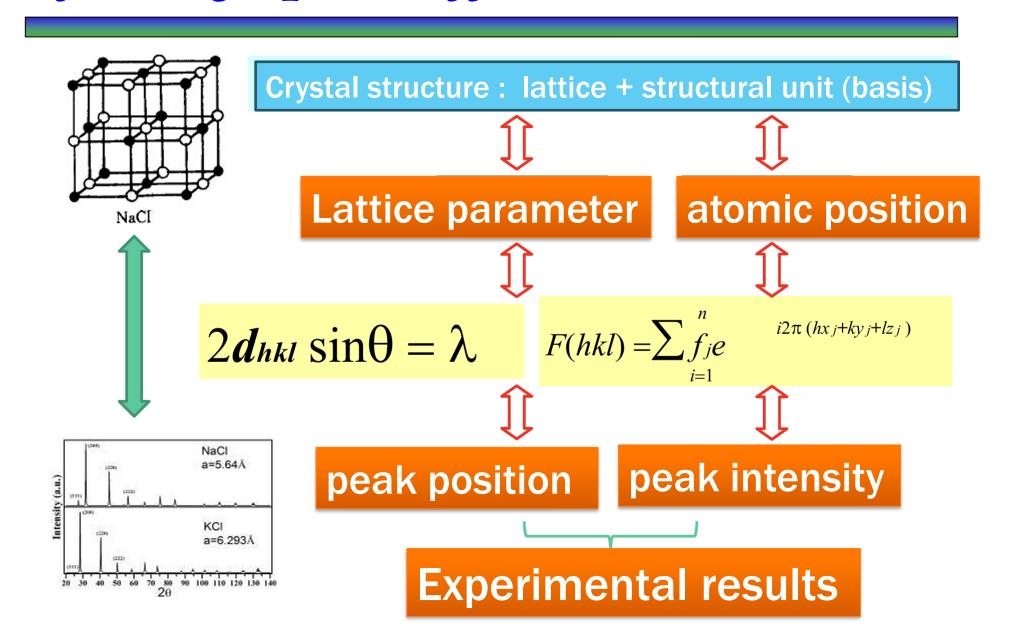


# X-ray diffraction - interference of coherent scattering

Each electron in the material is subjected to vibration under the action of the electric field of X-rays. In this way, the electrons generate electromagnetic waves of the same frequency as the incoming X-rays in all directions, and the interference between the coherent scattering from the long-range neighboring lattices causes X-ray diffraction.



# X-ray Crystallographic Diffraction Structure Analysis

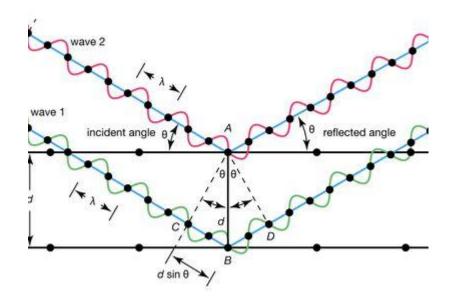


# Bragg equation

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

•Incident beam and lattice parameters:

 $\theta$  d a, b, c,  $\alpha$ ,  $\beta$   $\gamma$ 



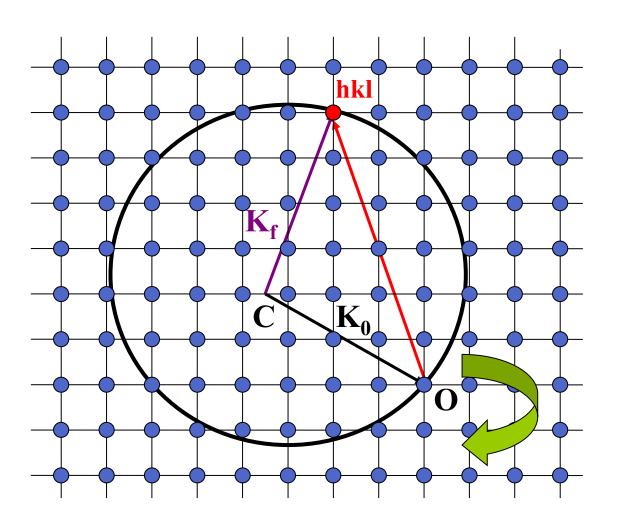
#### Interplanar spacing, for Orthorhombic lattice

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

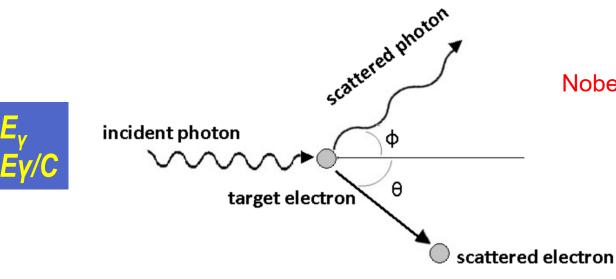
Determine the position of the diffraction peak, the diffraction spectrum is the change of the diffraction intensity with the angle  $\theta$ , or the change of the diffraction vector q, the diffraction angle and the wavelength:  $q=4\pi\sin\theta/\lambda$ 

# Ewald sphere

When a reciprocal lattice point intersects the Ewald sphere, it means the conditions defined by Bragg's law are met for that particular set of crystal planes. By rotating the crystal (and thus the reciprocal lattice) or changing wavelength of the incident X-rays, one can bring different reciprocal lattice points into contact with the Ewald sphere, resulting in diffraction from different crystal planes.



# Compton scattering (incoherent scattering)



E<sub>e</sub>

Nobel Prize in Physics 1927

Conservation of energy:

$$E_{\gamma} = E_{\gamma'} + E_{e}$$

$$\frac{E_{\gamma}}{c} = \frac{E_{\gamma'}}{c}\cos\theta + p\cos\phi$$

$$\frac{E_{\gamma'}}{c}\sin\theta = p\sin\phi$$

$$E_e^2 = E_0^2 + p^2 c^2$$

$$E_0 = m_e c^2$$

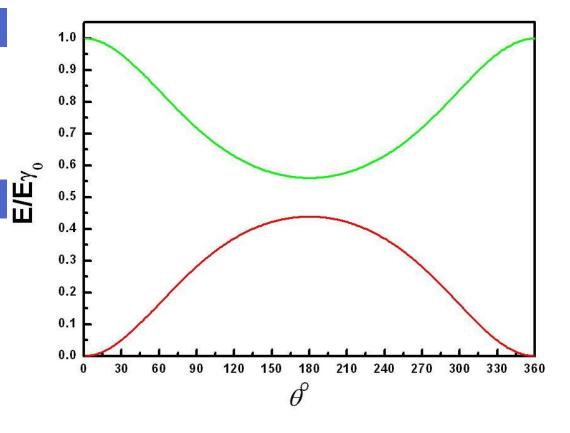
# Compton scattering

#### Photon energy angular distribution:

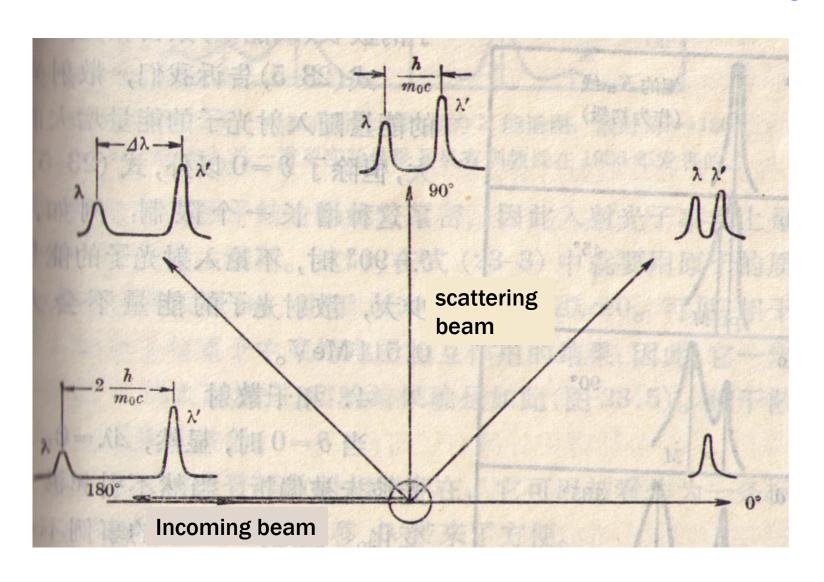
$$hv' = \frac{hv}{1 + \frac{hv}{mc^2}(1 - \cos\theta)}$$

#### electron energy angular distribution:

$$E_e = \frac{h\nu(1-\cos\theta)}{\frac{m_0c^2}{h\nu} + (1-\cos\theta)}$$



# Compton scattering



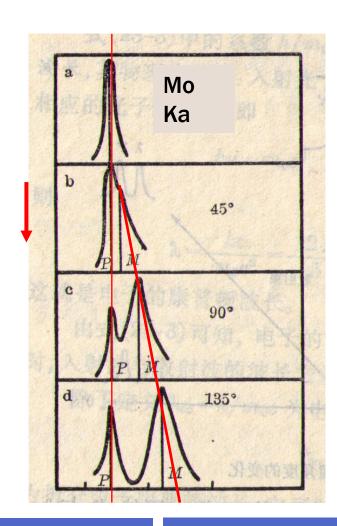
$$\Delta \lambda = \lambda' - \lambda = \frac{h}{m_0 c} (1 - \cos \theta)$$

$$\theta = 180^{\circ}$$

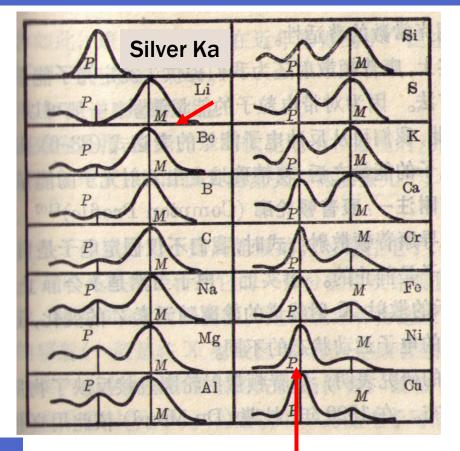
$$\Delta \lambda_{\text{max}} = \frac{2h}{m_0 c} = 0.049 \, \mathring{A}$$

$$E_{k,\text{max}} = \frac{2\frac{hv}{m_0 c^2}}{1 + 2\frac{hv}{m_0 c^2}} hv$$

# Compton scattering



Coherent scattering: scattering of photons by inner shell electrons. Compton effect: scattering of photons by weakly bound electrons in the outer shell.



**Coherent scattering** Compton Scattering

The larger the Z, the stronger the coherent scattering

# **Photoelectric effect**

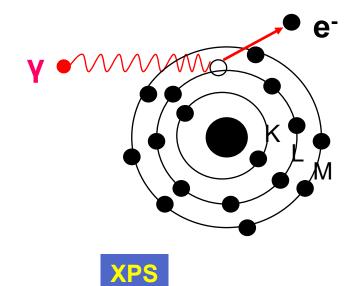
# Photoelectric effect

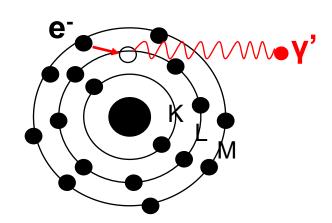
When the energy of a photon is greater than the binding energy of an electron in a certain orbit of an atom, the photon is absorbed by the electron, causing the electron of the atom to gain energy and become a free electron

**Photoelectron** kinetic energy:

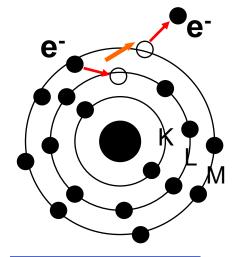
$$E_e = h \nu - E_B$$

$$E_B = R_c (Z - b)^2 (\frac{1}{n_i^2} - \frac{1}{n_j^2})$$
 $E_B = R_c (Z - b)^2 (\frac{1}{n_i^2} - \frac{1}{n_j^2})$ 
 $E_B = R_c (Z - b)^2 (\frac{1}{n_i^2} - \frac{1}{n_j^2})$ 
 $E_B = R_c (Z - b)^2 (\frac{1}{n_i^2} - \frac{1}{n_j^2})$ 
 $E_B = R_c (Z - b)^2 (\frac{1}{n_i^2} - \frac{1}{n_j^2})$ 



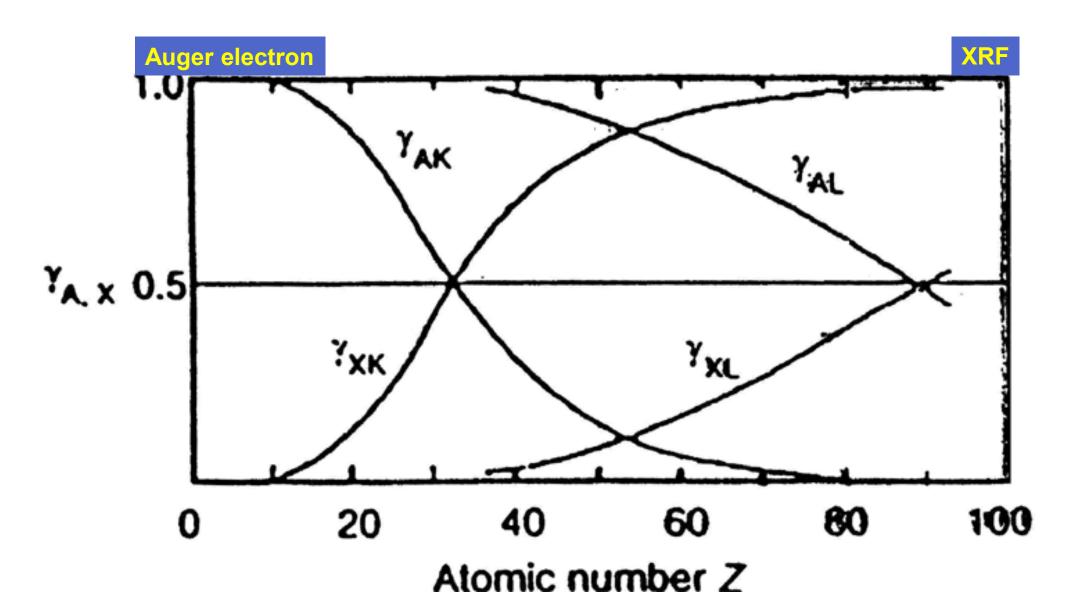




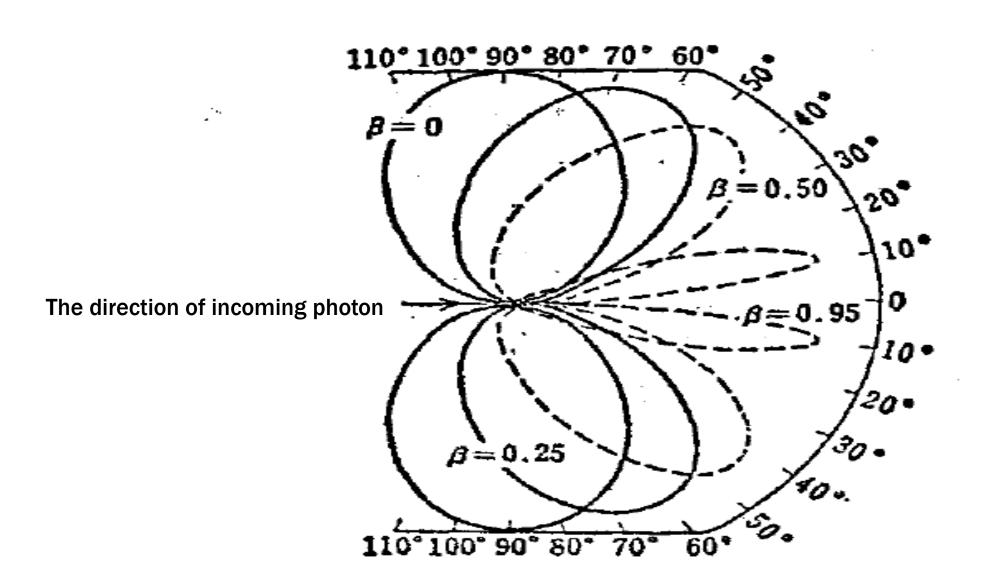


**Auger electron** 

## Competition between the two secondary effects of the photoelectric effect

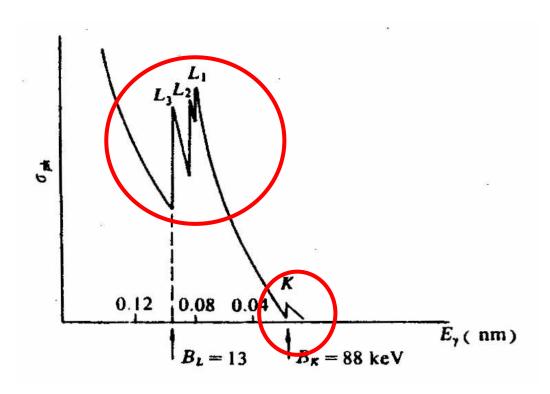


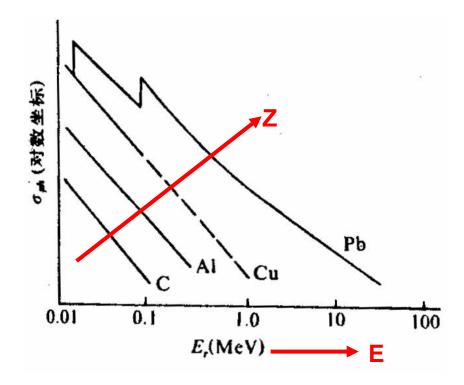
# Angular distribution of photoelectrons



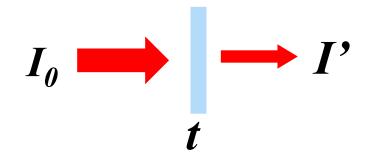
# Photoelectric effect cross section

cross section: the probability of interaction between microscopic particles: the probability of a particle colliding with another particle in a unit area perpendicular to the direction of motion per unit time. A geometric cross section equivalent to the probability of collision.





# X-ray attenuation (absorption) in matter



#### Photoelectric effect, scattering (including Compton effect), electron pair effect...

$$\frac{I' - I_0}{I_0} = \frac{dI}{I_0} = -\mu t$$

$$I = I_0 \exp(-\mu t)$$

$$\mu = \mu_{ph} + \mu_c + \mu_p$$

# Linear Absorption Coefficient and Mass Absorption Coefficient

The attenuation of X-rays (Compton scattering, photoelectric effect, electron pairs) is related to the total number of interacting atoms (electrons) and has nothing to do with their morphology (density).

$$\mu_m = \frac{\mu}{\rho}$$

$$I = I_0 \exp(-\mu t) = I_0 \exp\left(-\frac{\mu}{\rho} \cdot \rho t\right) = I_0 \exp(-\mu_m t_m)$$

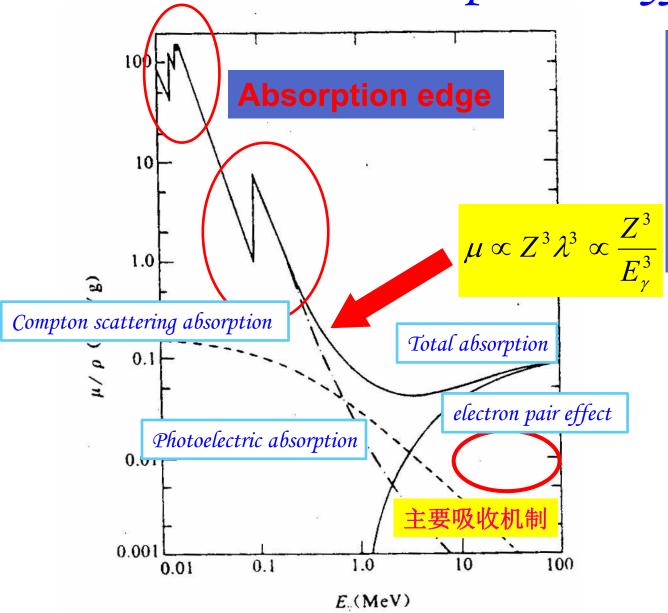
#### compound or mixture

Mass absorption coefficient Mass thickness:

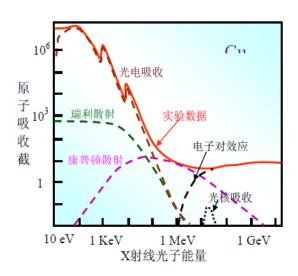
$$\mu_m = \sum_{i=1}^n w_i \mu_{mi}$$
 The weighted sum of each component  $t_m = \rho t$ 

$$t_m = \rho t$$

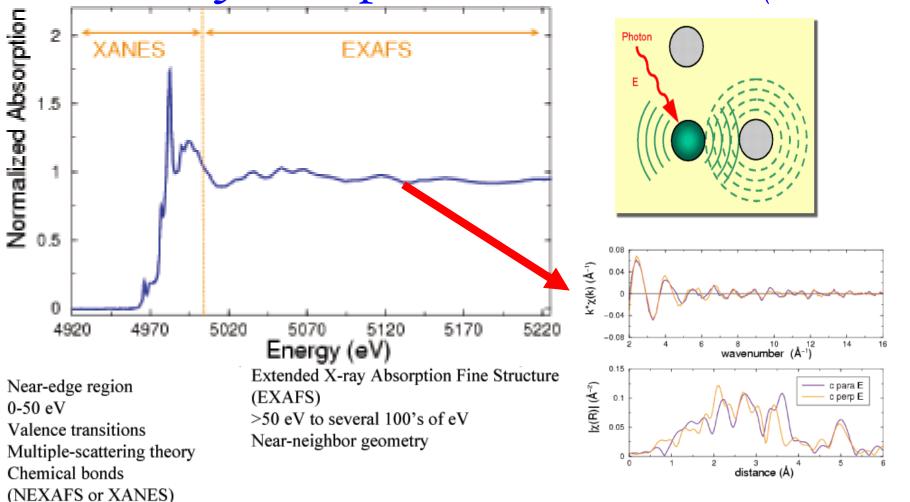
# Absorption coefficient



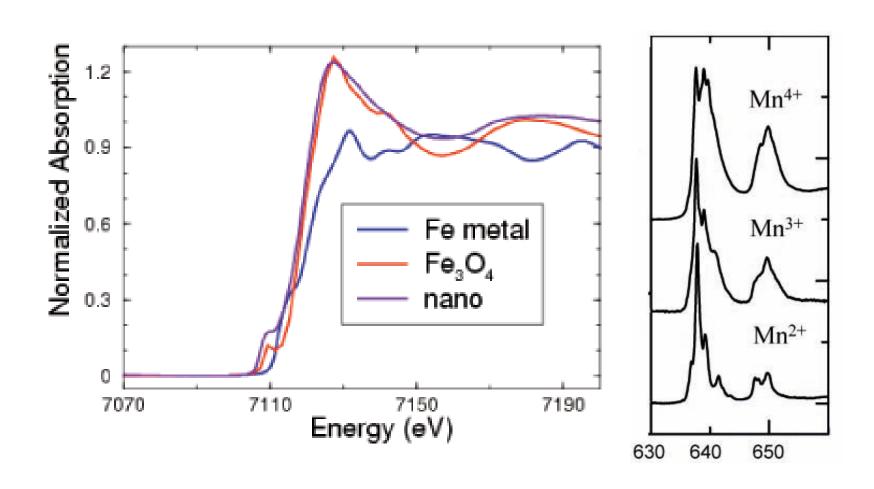
- X-ray absorption spectroscopy: XAS
- Extended X-ray absorption fine spectroscopy: XAFS
- X-ray near-edge absorption spectroscopy: XANSE



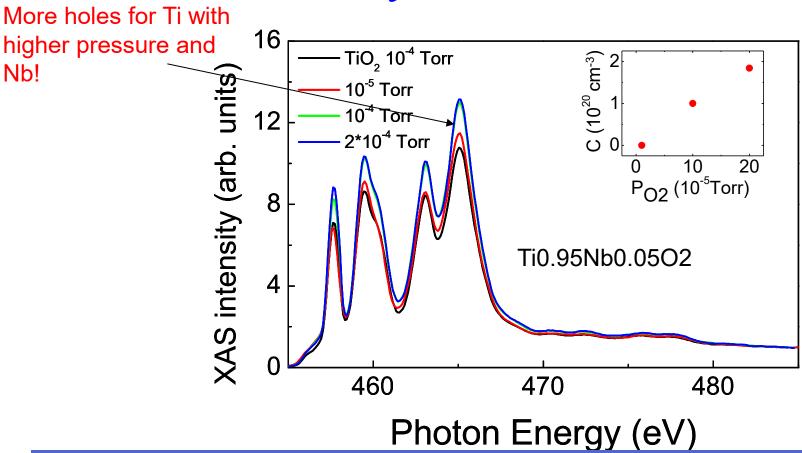
X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS)



## XANES



#### XANES

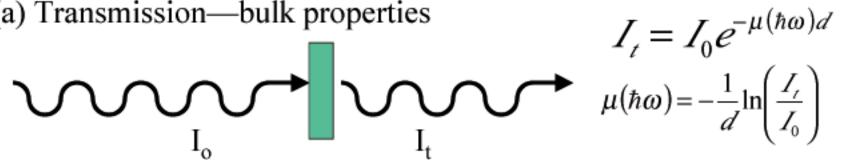


Ti L edge XAS spectra for different TiO2 films. The inset: the concentration of magnetic moment vs oxygen partial pressure.

Adv. Mater., 21, 2282, (2009).

## Different detection modes

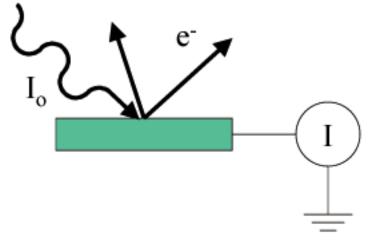
(a) Transmission—bulk properties



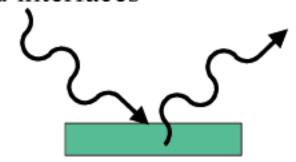
$$I_t = I_0 e^{-\mu(\hbar\omega)d}$$

$$\mu(\hbar\omega) = -\frac{1}{d} \ln \left( \frac{I_r}{I_0} \right)$$

(b) Total electron yield —surface properties

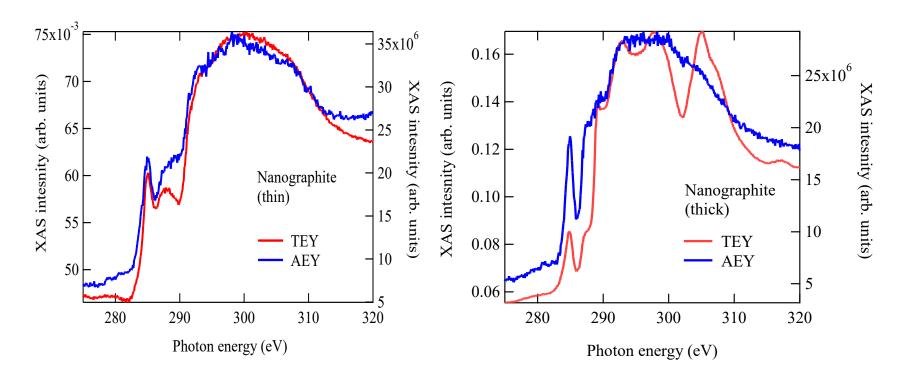


(c) Fluorescence—dilute species; Buried interfaces



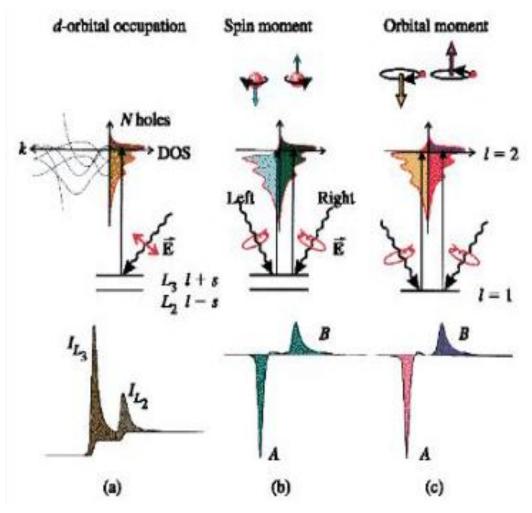
Different surface sensitivity!

# Nanographite: chemical states at different depths



C K-edge XANES spectra of one kind of nanographite at different thicknesses

# XMCD (x-ray magnetic circular dichroism)



**Dipole selection rules** 

For left-circular

$$\Delta_{\rm ml} = -1$$
$$\Delta_{\rm ms} = 0$$

For right-circular

$$\Delta_{ml} = +1$$
  
 $\Delta_{ms} = 0$ 

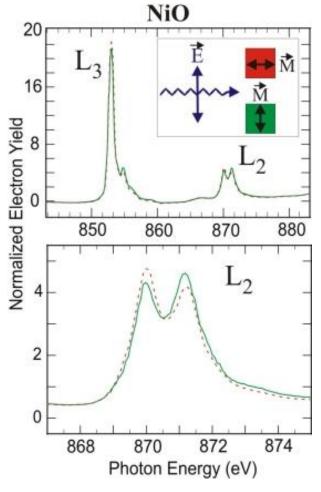
#### **Sum Rules**

$$M_{spin} = C(A - 2B)$$
 Spin moment

$$M_{orb} = C(A + B)$$
 Orbital moment

C total intensity (number of d-holes)

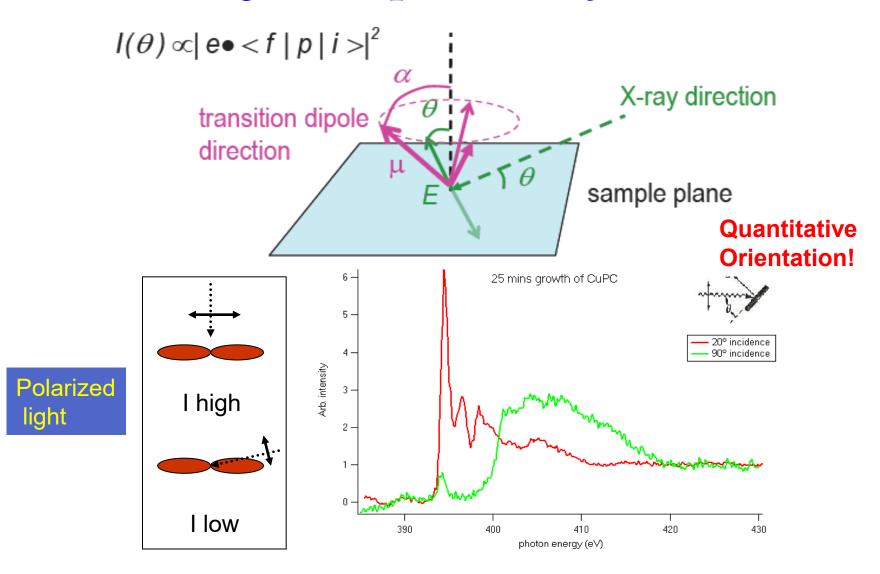
# X-ray magnetic linear dichroism (XMLD)



10A Pt 12A Co LaFeO<sub>3</sub>(100) LaFeO<sub>3</sub> layer Co layer 710 720 730 770 780 790 800 Photon Energy (eV)

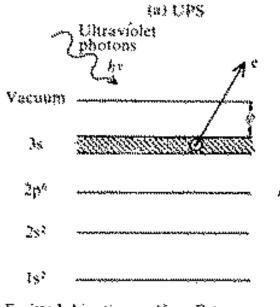
Only sensitive to spin along which axis!

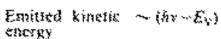
# Angular dependence of XANES

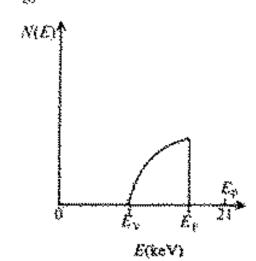


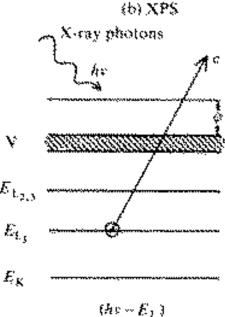
# Electron spectroscopies: photoemission

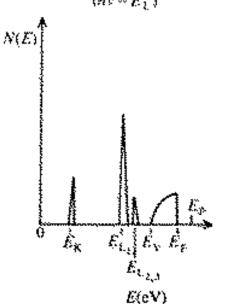
- XPS (X ray photoemission spectroscopy)
   /ESCA (Electron Spectroscopy for Chemical Analysis)
- Ultraviolet Photoelectron Spectroscopy (UPS)
- Auger electron spectroscopy

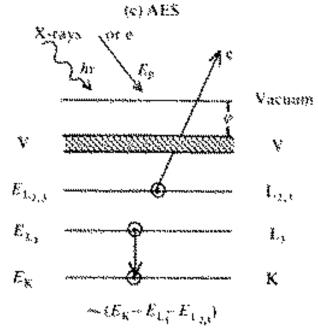


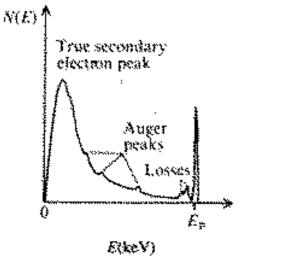




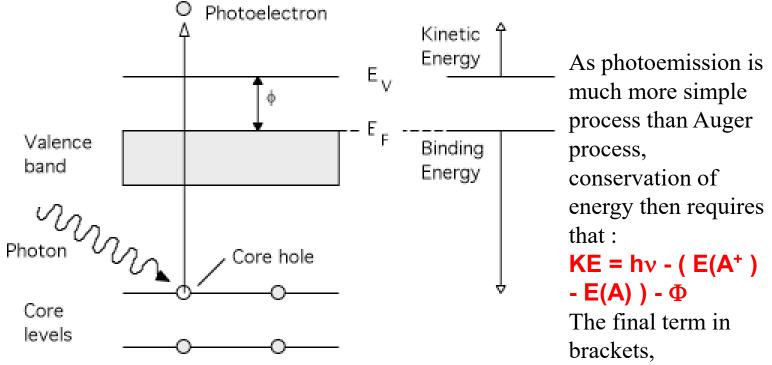








#### Theoretical consideration

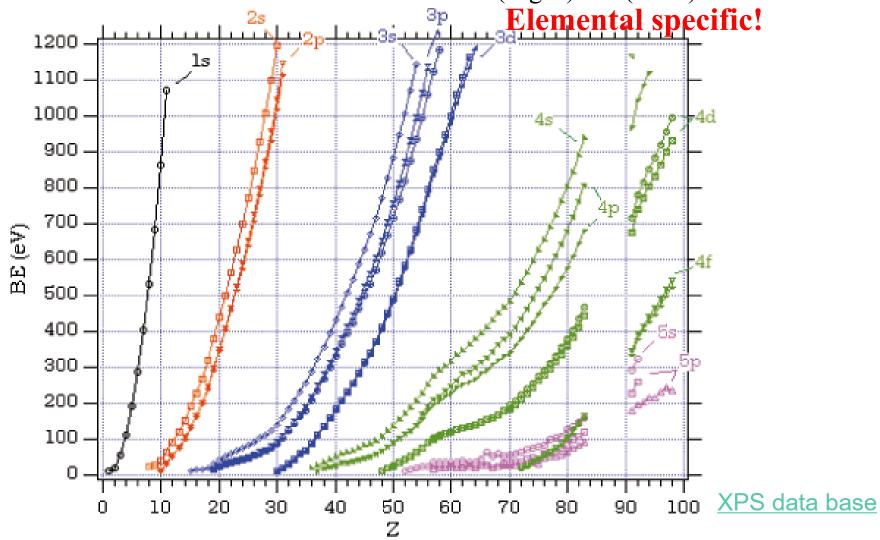


representing the difference in energy between the ionized and neutral atoms, is generally called the *binding energy* (BE) of the electron. ( $\Phi$  is the work function of the solid when KE is counted near surface, however, KE detected by analyzer then  $\Phi$  is the work function of analyzer.)

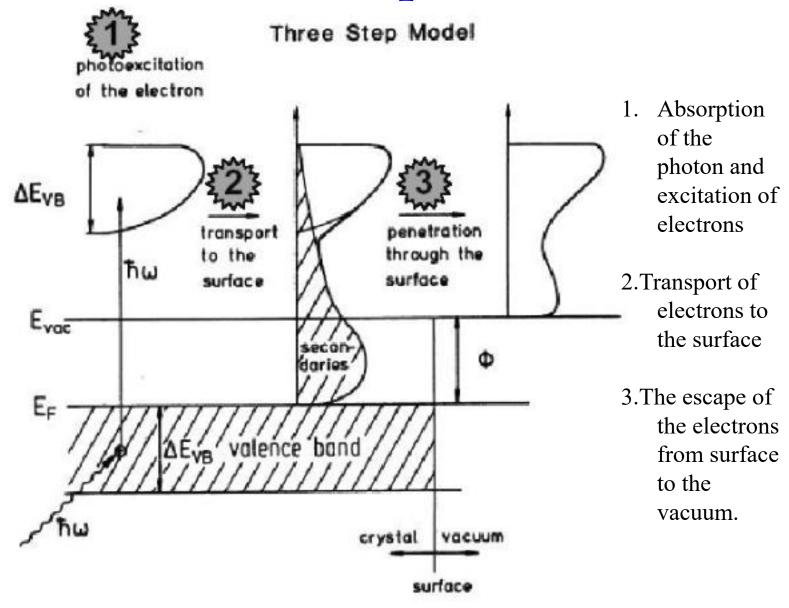
# Z dependence

BE follows the energy levels: BE(1s)>BE(2s)>BE(2p)...

BE with same orbital increase with Z: BE(Mg1s)>BE(Na1s)

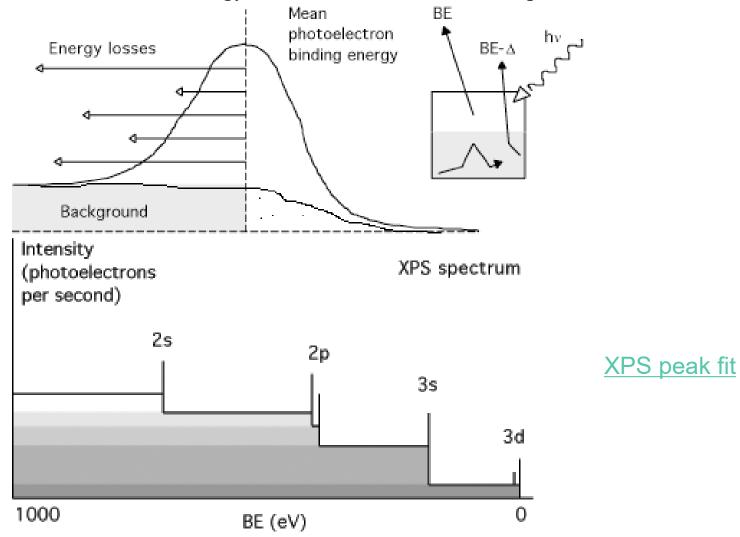


# Three Step Model

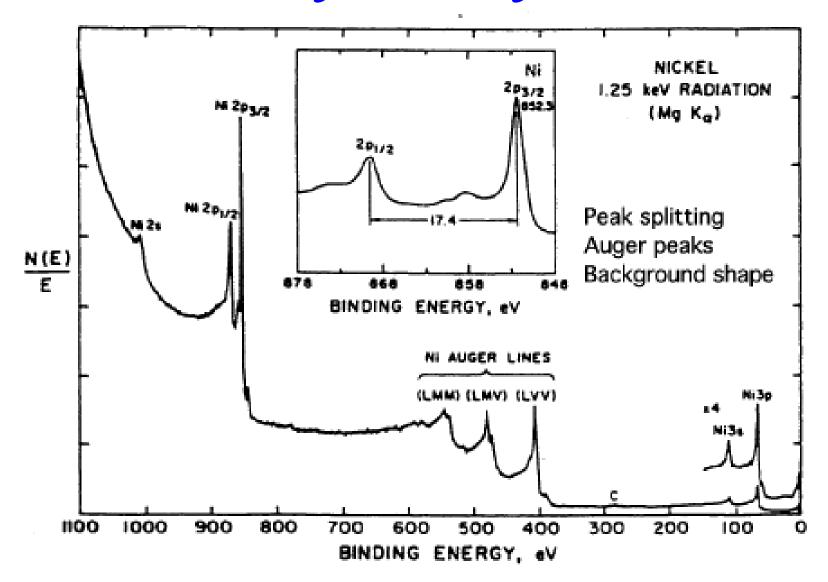


# Inelastic scattering

In the step 2, inelastic scattering let XPS spectra consists of core-level photoemission peaks imposed by a step-like structure (background) due to the various mechanism to lose kinetic energy. Besides, there are also AES processes visible.



# Main features of XPS



# Core Level Chemical Shifts

Position of orbitals in atom is sensitive to chemical environment of atom. In solid all core levels for that atom shifted by approx. same amount (<10 eV). Chemical shift correlated with *overall charge* on atom (Reduced charge ®increased BE)

For k-shell of an atom in a compound:

$$E_B(k) = E_B(k,q_A) + V$$

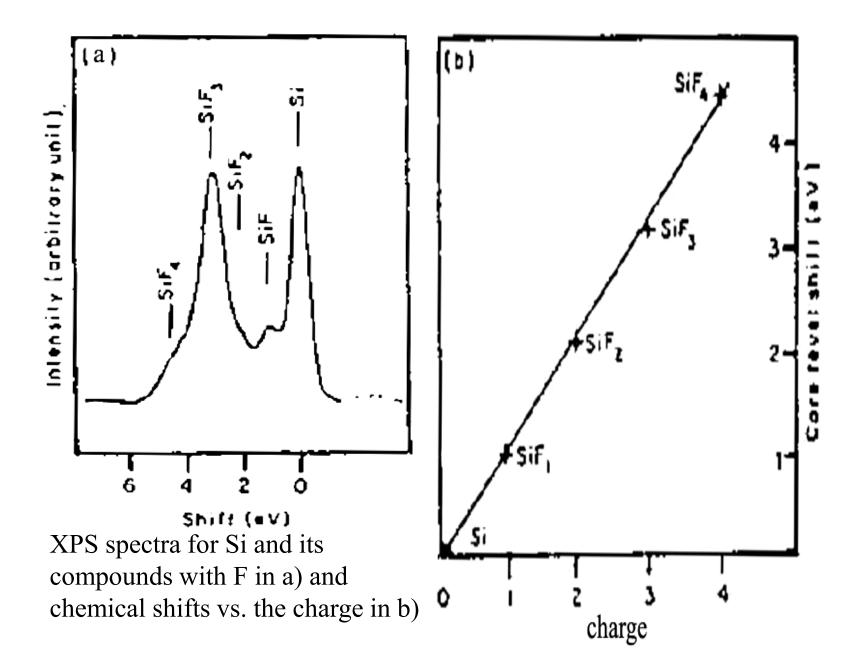
where  $E_B(k,q_A)$  is the binding energy of a free ion, A, qA is the net charge of A, and V is the potential at A due to all other atoms. V can be described as:

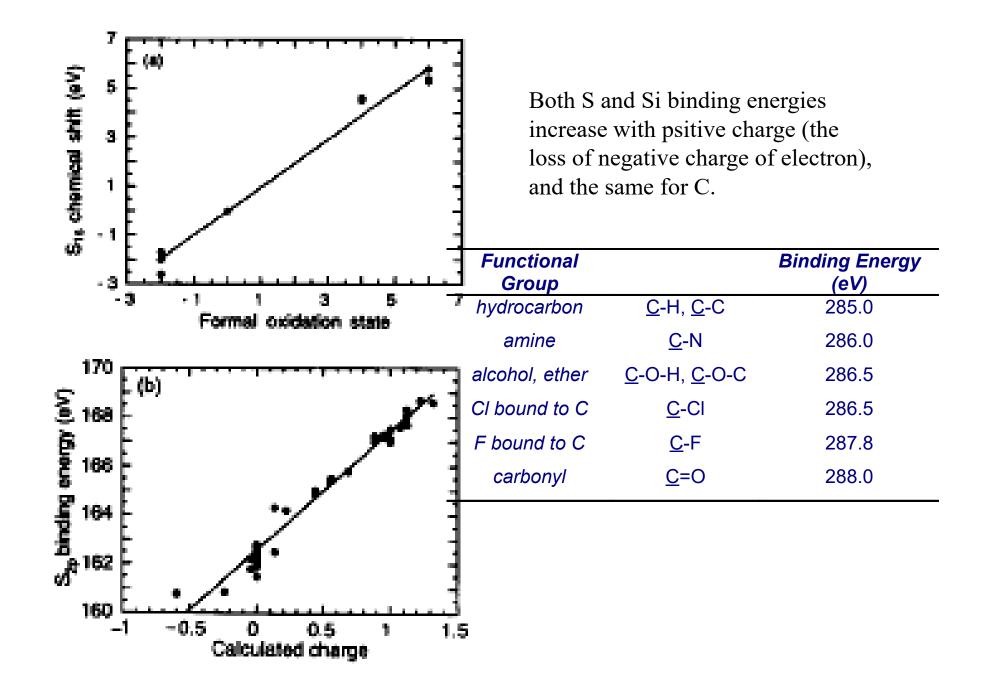
$$V = e^2 q_A \Sigma q_i / r_{iA}$$

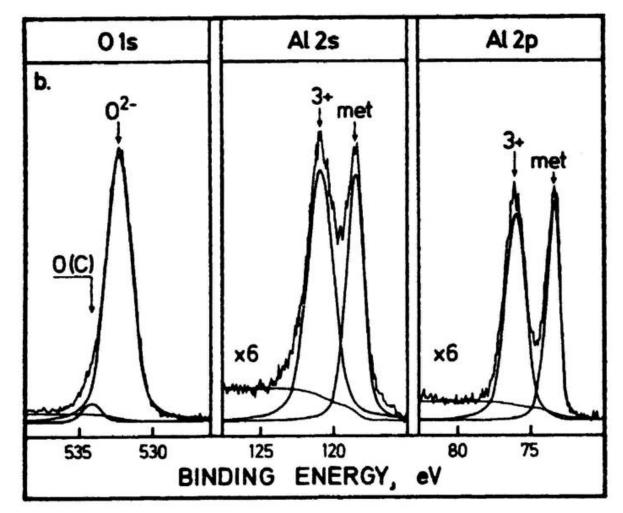
(i is any other atoms except A),  $\mathbf{r}_{iA}$  is the distance between i and A, therefore chemical shift is:

$$\Delta E_B(k) = E_B(k, q_{A1}) - E_B(k, q_{A2}) + V_1 - V_2$$

 $\mathbf{q}_{A1}$  and  $\mathbf{q}_{A2}$  is the difference of charge in two states.







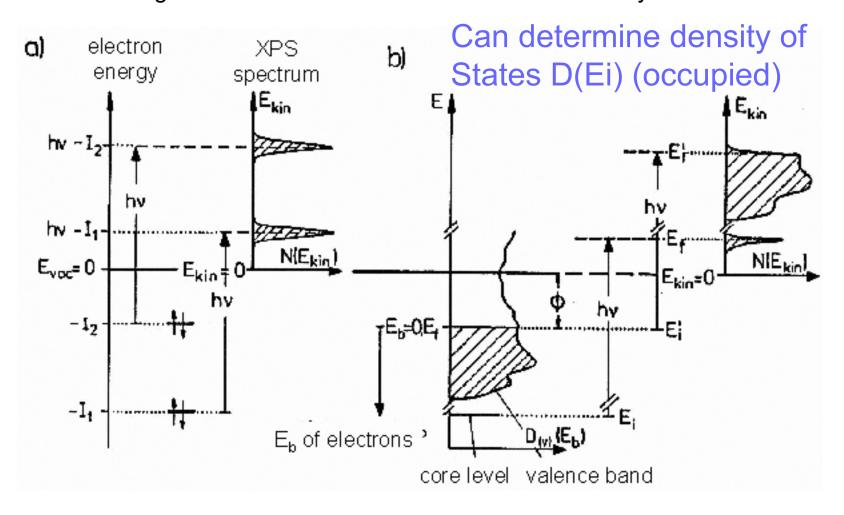
The chemical shifts due to the variation of the distribution of the charges at the atom site is the main reason for the other name of XPS:

ESCA
(Electron
Spectroscopy for
Chemical Analysis)

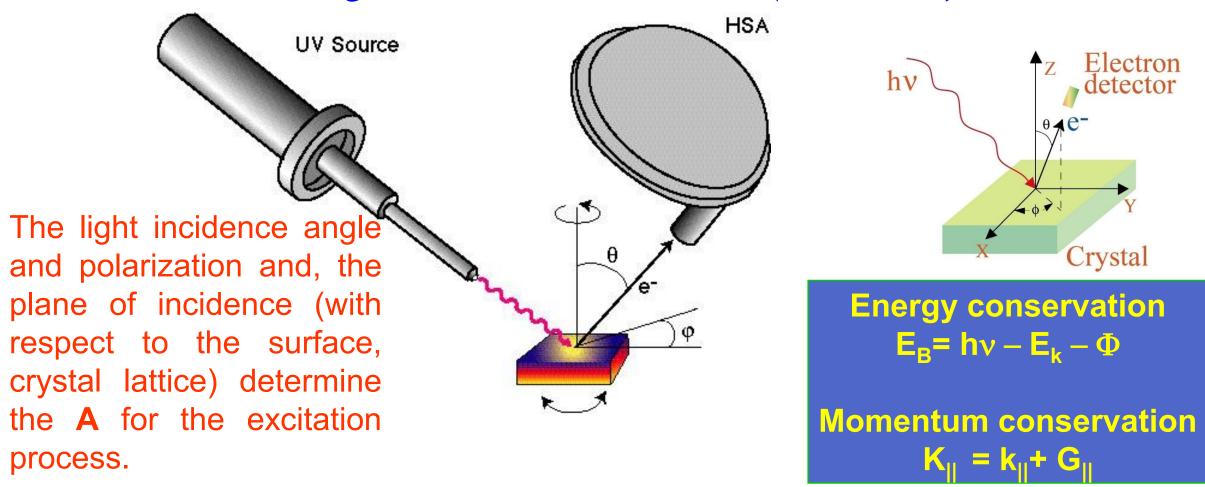
As the samples shown before, binding energies of Al<sup>3+</sup> is higher than the metal atom, in the meanwhile, the binding energy of O atom (more positive charge) is higher than the O<sup>2-</sup> ion.

# Ultraviolet Photoelectron Spectroscopy (UPS)

UV light (hv = 5 to 100 eV) to excite photoelectron. From an analysis of the kinetic energy and angular distribution of the photoelectrons, information on the **electronic structure** (band structure) of the material under investigation can be extracted with surface sensitivity.



# Angular Resolved UPS (ARUPS)



UPS spectra also have strong angular dependence for the excited electron, which can give information about band structure in the k space.

# Imaging

Scanning

Zone Plate Focusing Lens

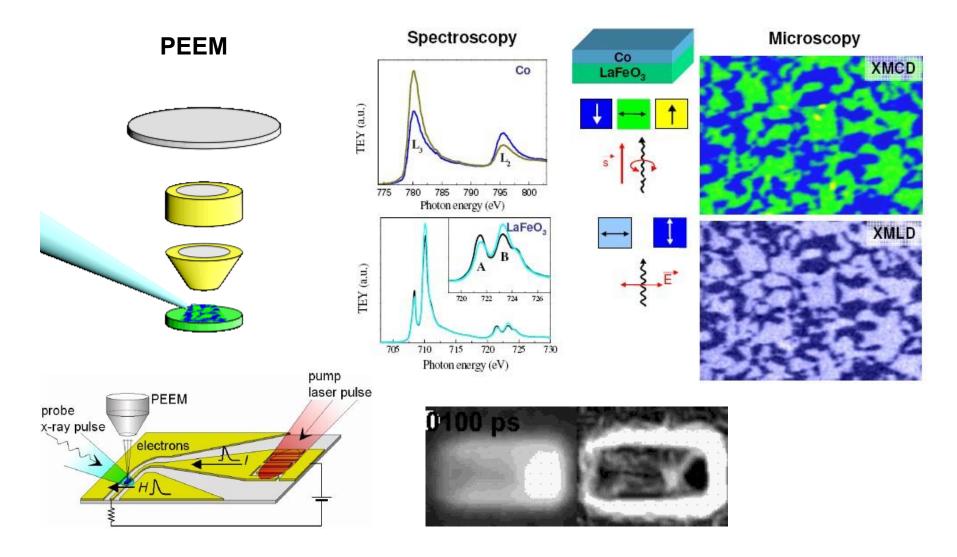




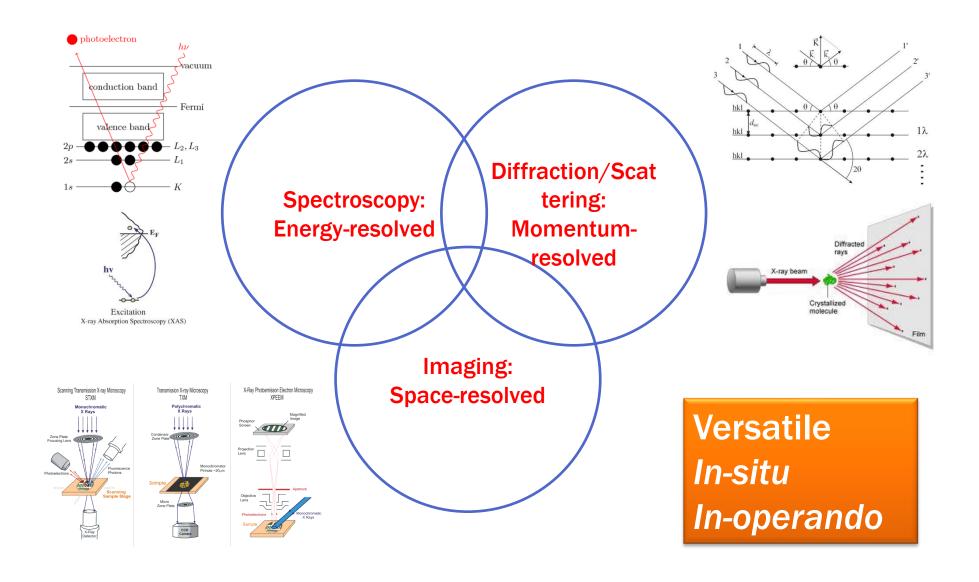


MicroCT

# Different contrasts



# Synchrotron-based techniques

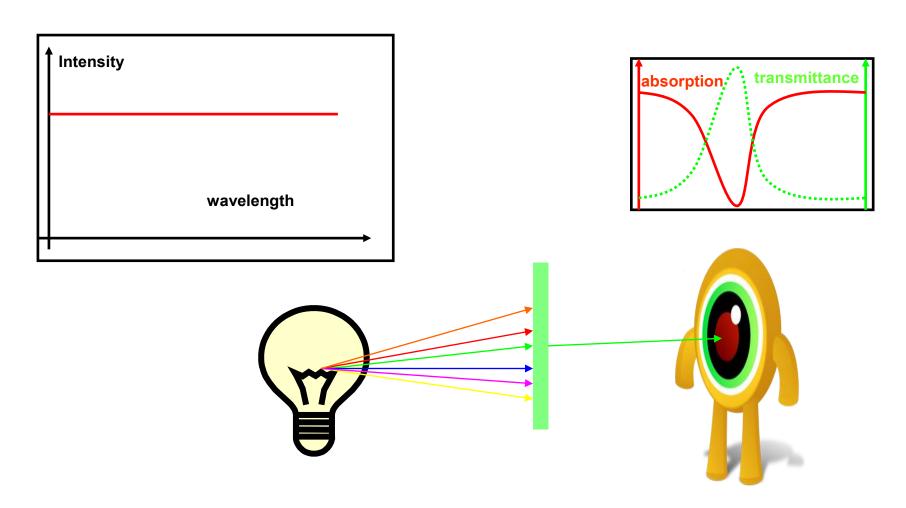


03

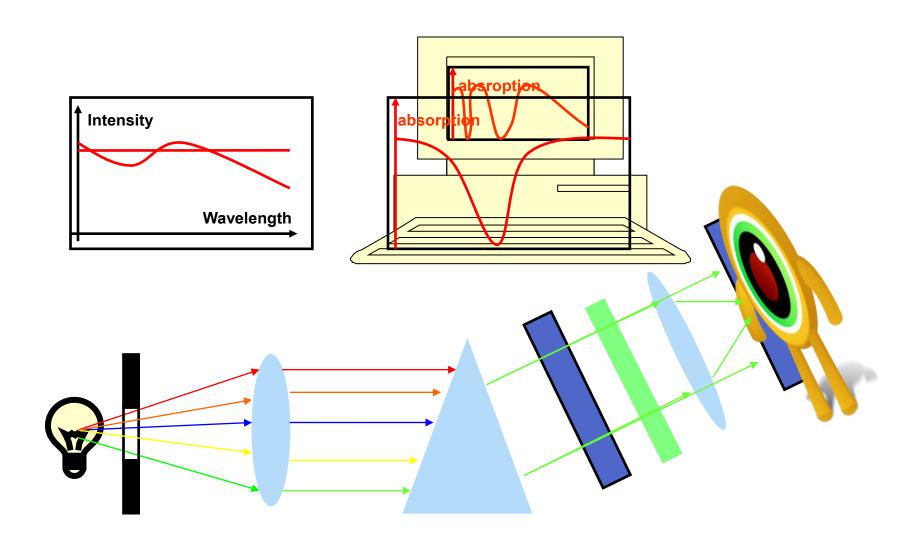
# Synchrotron beamlines



# Functions of the beamlines



# Functions of the beamlines



#### Key information about beamlines

#### The study objects/ scientific goals

single crystals, polycrystalline powders, surfaces and interfaces of thin films/ultra-thin films, microstructures of nanomaterials

**Crystal structure** analysis: crystal structure, crystal constant determination; Phase analysis: qualitative and quantitative analysis of phase (intensity ratio); Grain size; Crystallinity analysis; Stress analysis;Thin film thickness; Reflectivity; **Preferred orientation** and texture analysis;

# **Experimental techniques**

- Conventional single crystal or powder X-ray diffraction (XRD)
- Grazing incidence X-ray (anomalous) diffraction (GIXRD/GIXAD)
- X-ray reflectivity measurement (XRR)
- Reciprocal space intensity distribution measurement (RSM)
- Diffraction anomalous fine structure (DAFS)
- Multi-wavelength anomalous diffraction (MAD)

#### **Specifications**

Energy range 4-10 keV

**Energy resolution** 

ΔE/E ~ 1.5×10<sup>-4</sup>@ 10keV

Spot size

 $\sim 0.35$  (H)  $\times 2.5$  (V) mm<sup>2</sup>

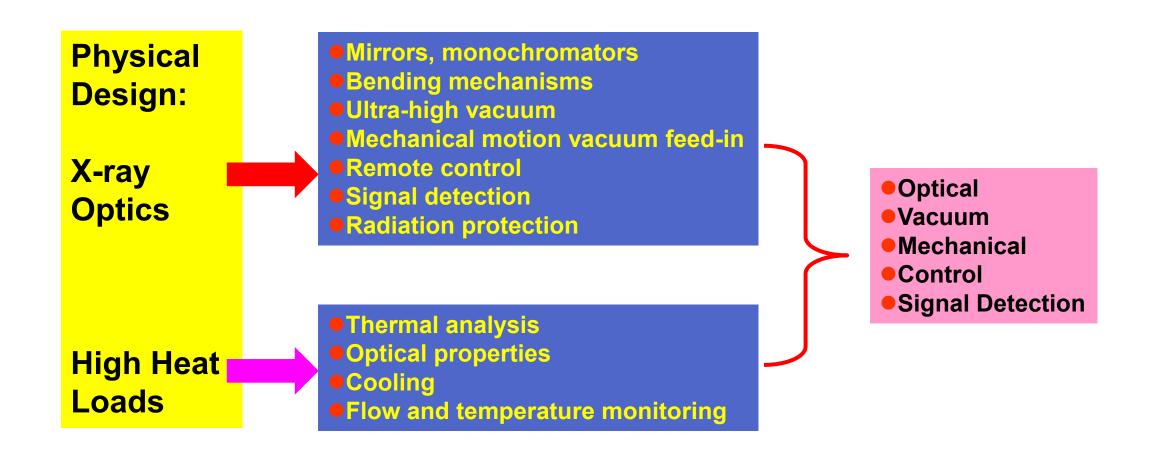
**Photon flux** 

~ 1.0×10<sup>12</sup> phs/s @ 10 keV

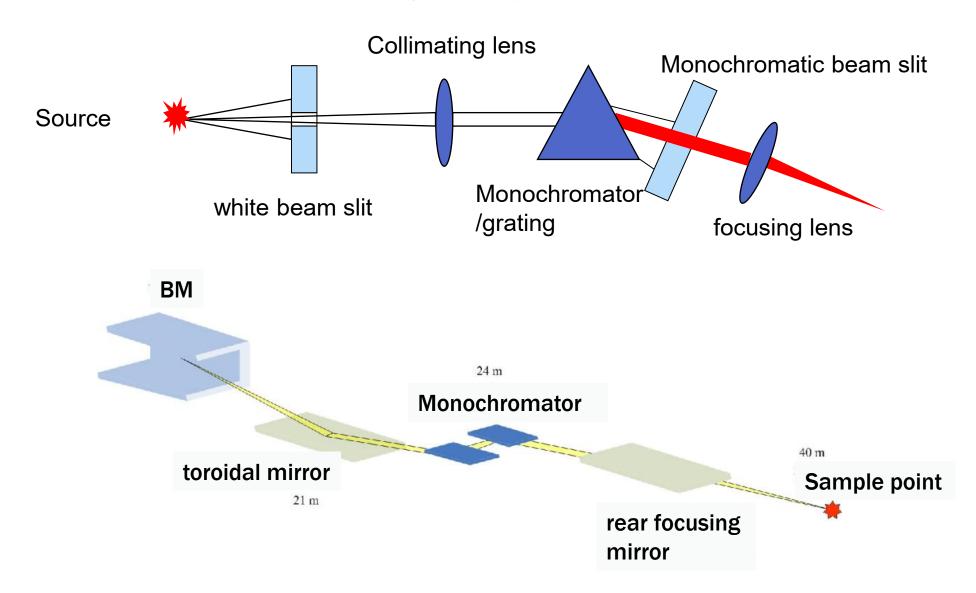
**Divergence angle** 

~ 2.5 (H)  $\times 0.02$  (V) mrad<sup>2</sup>

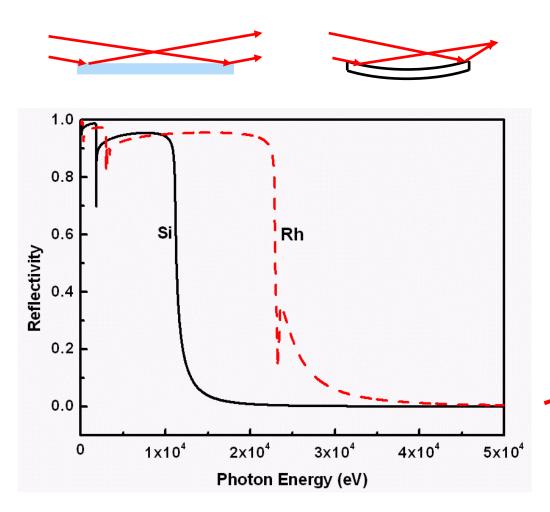
### Design and construction of beamlines

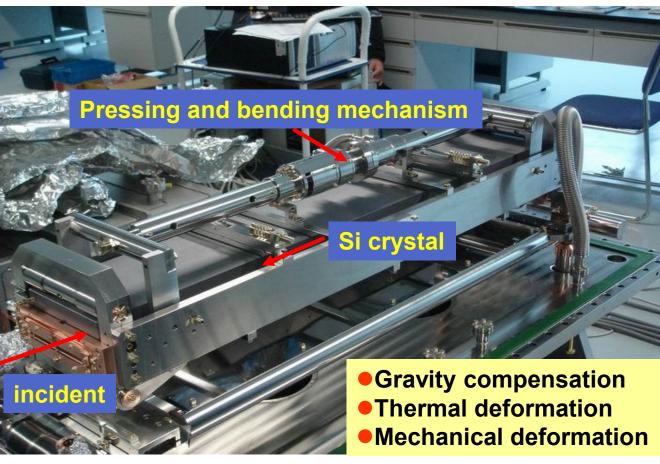


## Optical layout of a beamline

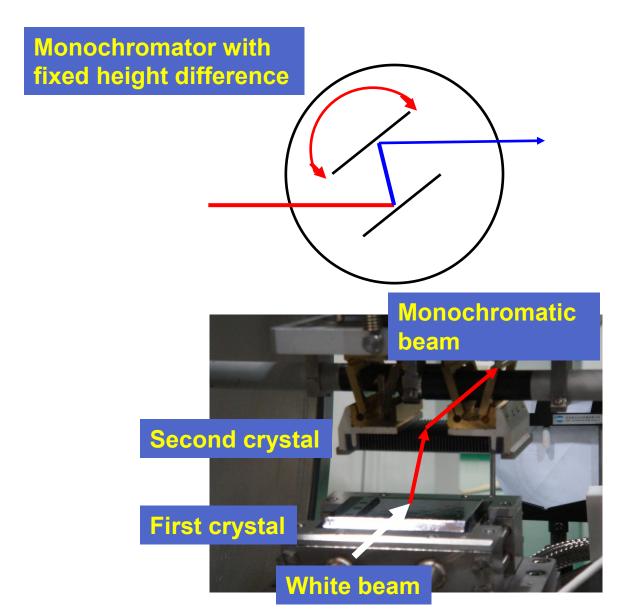


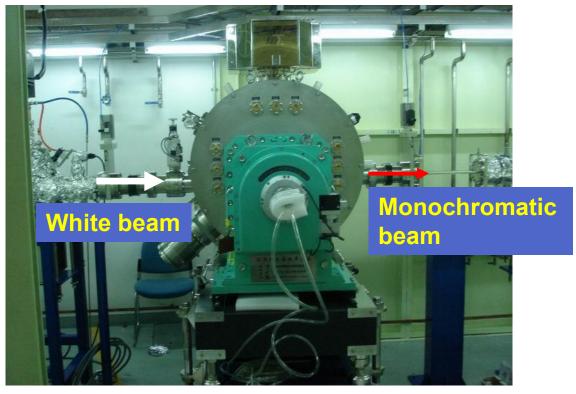
### Reflection and focus



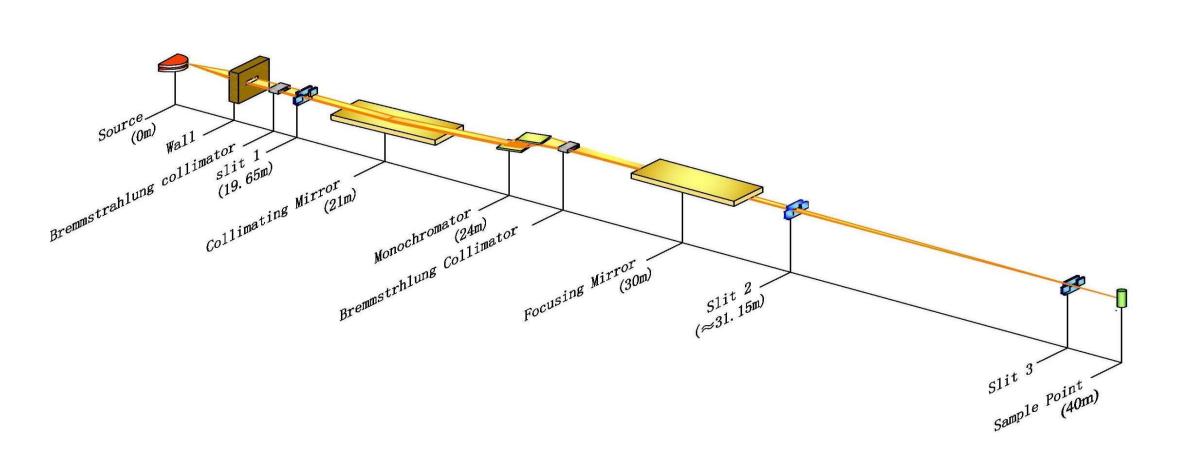


#### Monochromator





# The optical layout



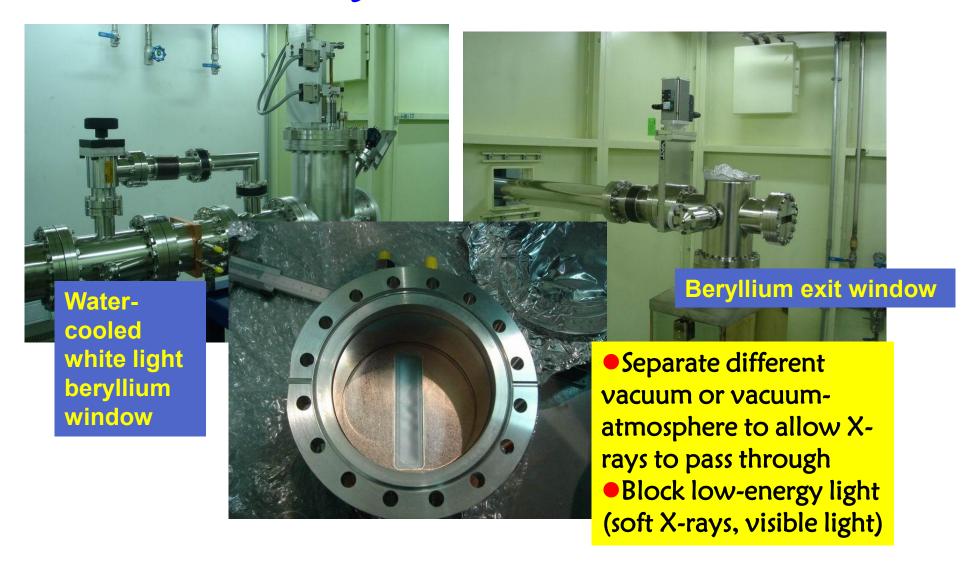
#### White beam slit



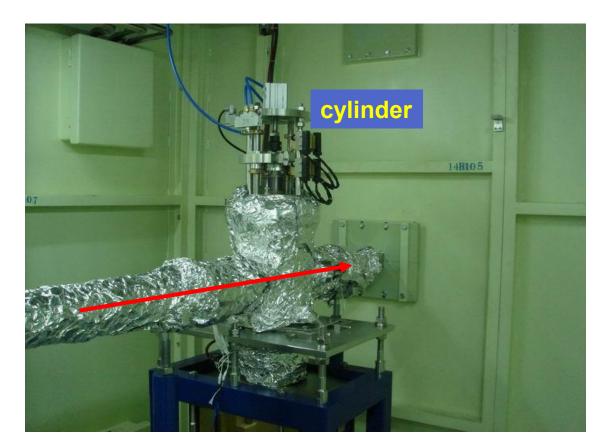
Two pairs of blades along vertical and horizontal directions

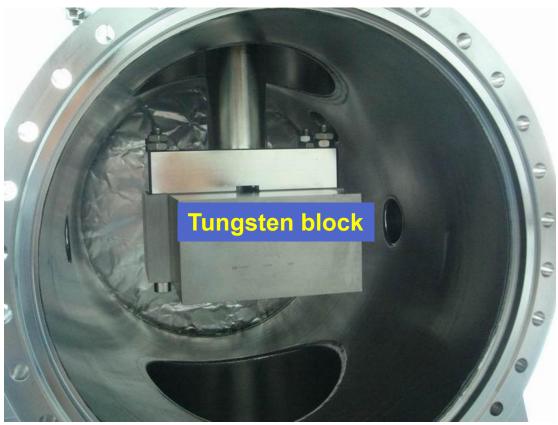
Control incident beam size

## Beryllium Window



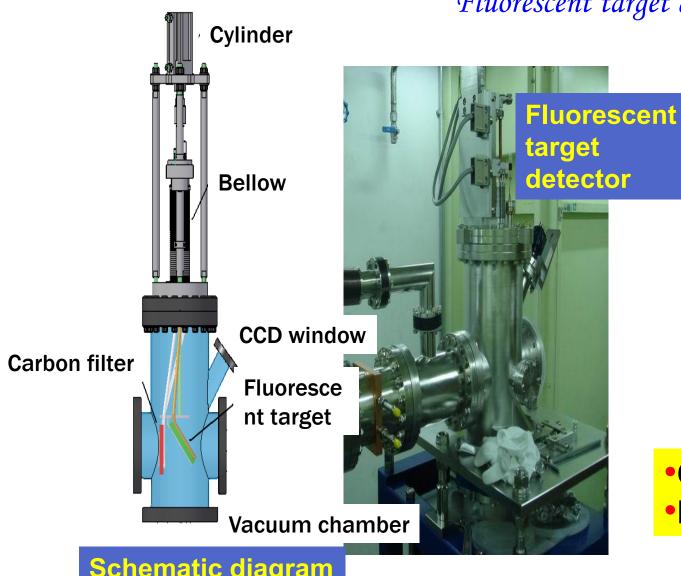
# Safety shutter

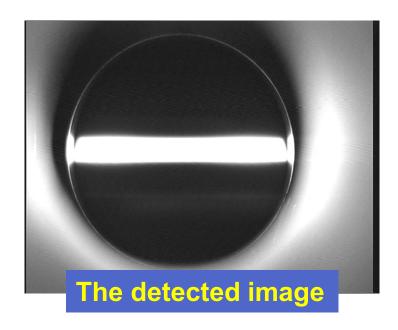




**Blocking synchrotron radiation** 

#### Fluorescent target detector

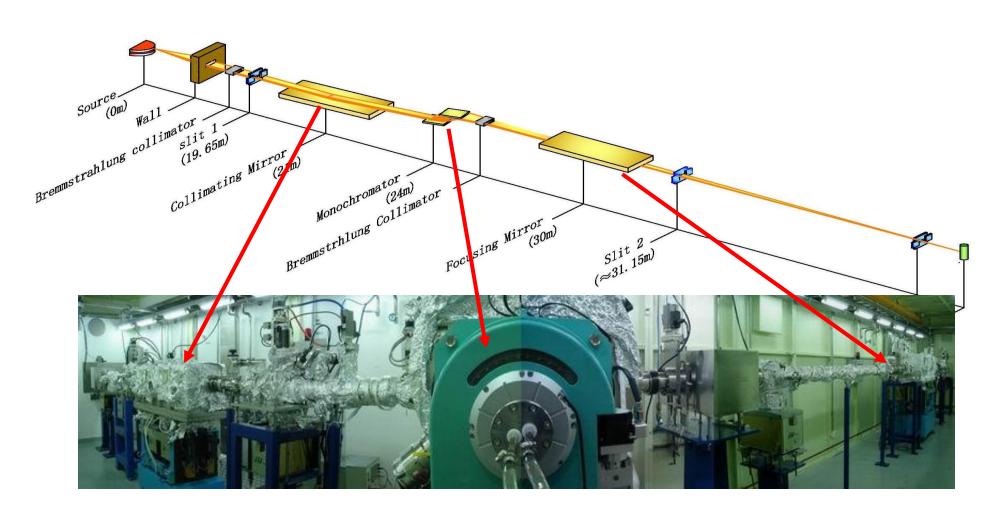




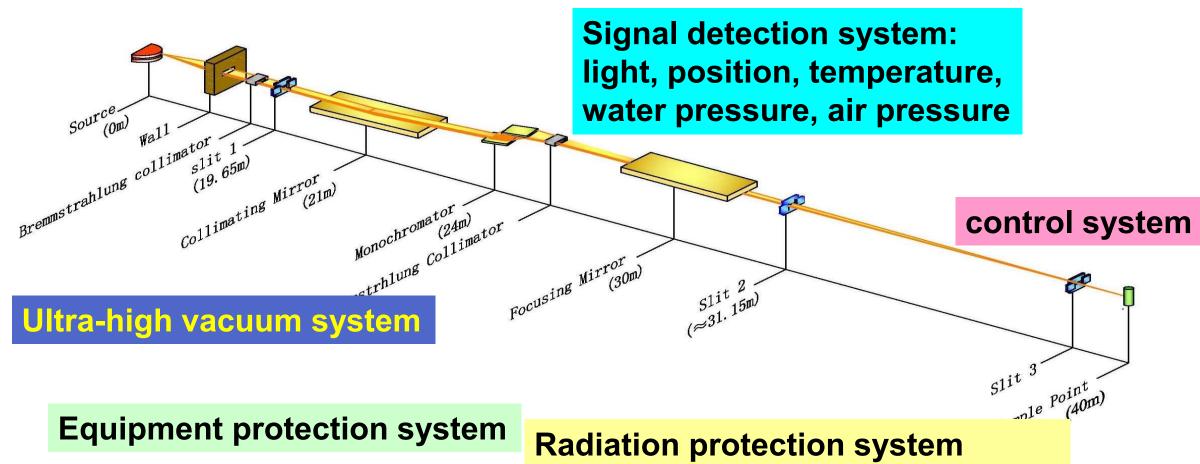
- Observing the beam shape
- Estimating the beam position

**Schematic diagram** 

# Photo of the beamline



## Beamline configuration



Radiation protection system Personal safety protection system

## Beamline control system



Front-end control system



**Beamline Control Terminal** 

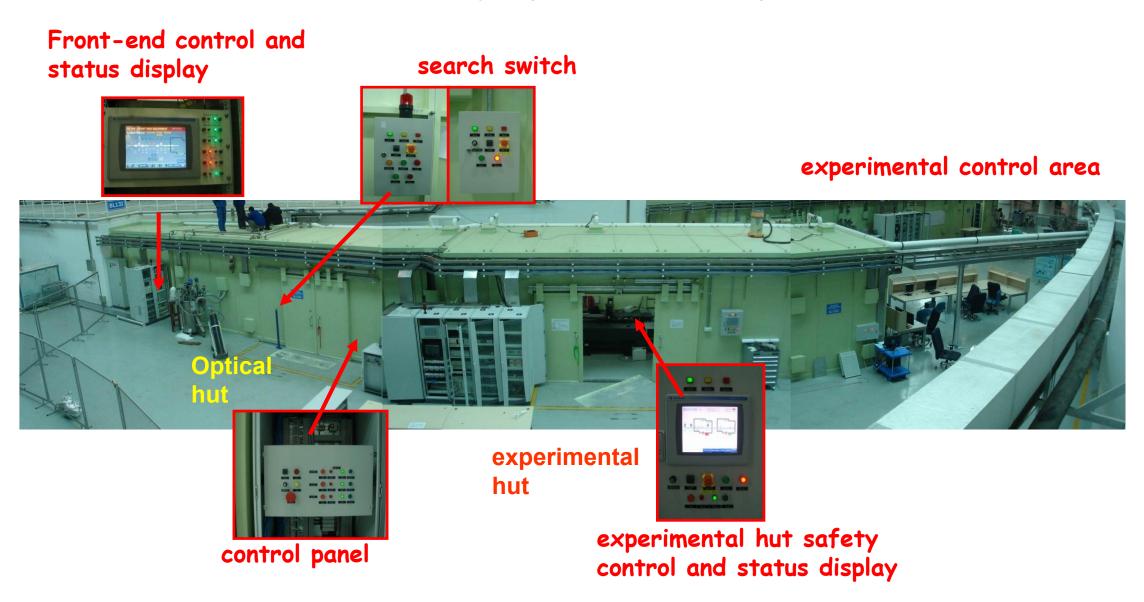
**Beamline control system** 

**Experimental station cabinet** 

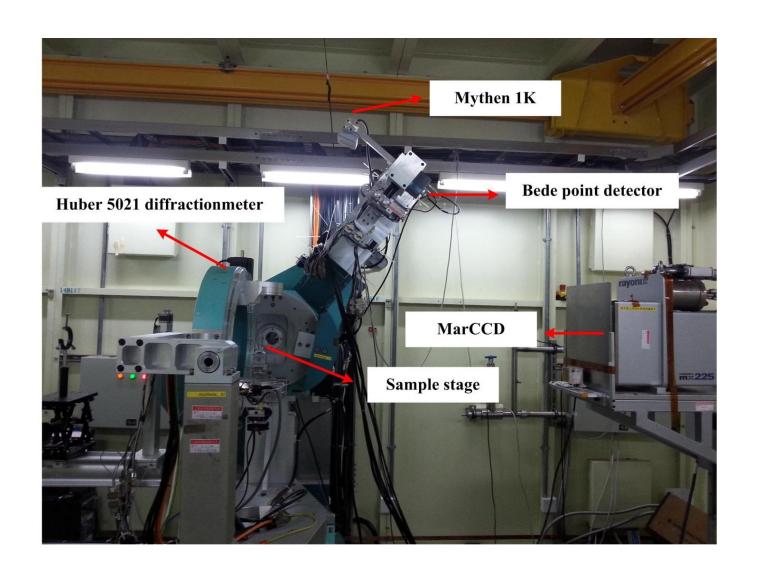
**Experimental area** 

**End station** 

## Personal safety protection system



## End station: diffractometer...



#### Beamline commission

#### **Spot size:**

X-ray CCD wire scanning

#### **Energy range**:

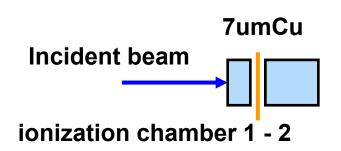
Monochromator scanning + ionization chamber measurement
Absorption edge

Light flux:

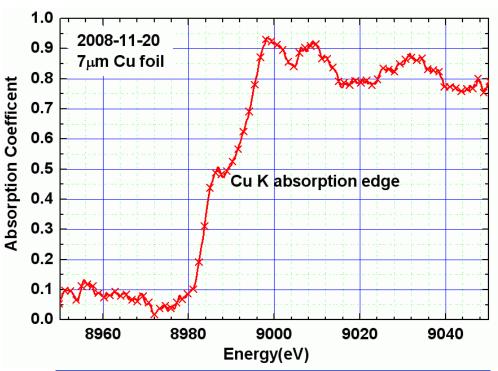
ionization chamber

#### **Energy resolution:**

**Absorption edge resolution Diffraction peak width** 







Clearly resolve the pre-peak: energy resolution <2.5eV

05

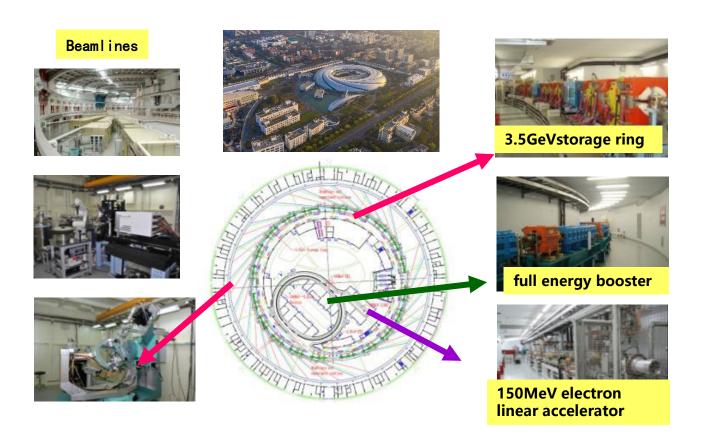
# Shanghai Synchrotron Radiation Facility (SSRF)



## SSRF overview

# A third generation synchrotron radiation light source, its overall performance ranks among the advanced levels of similar devices in the world.

A 150MeV electron linear accelerator, a full energy booster, a 3.5GeV storage ring and 34 beamlines with 46 end stations in operation.



**Electron energy: 3.5 GeV** 

Perimeter: 432 m

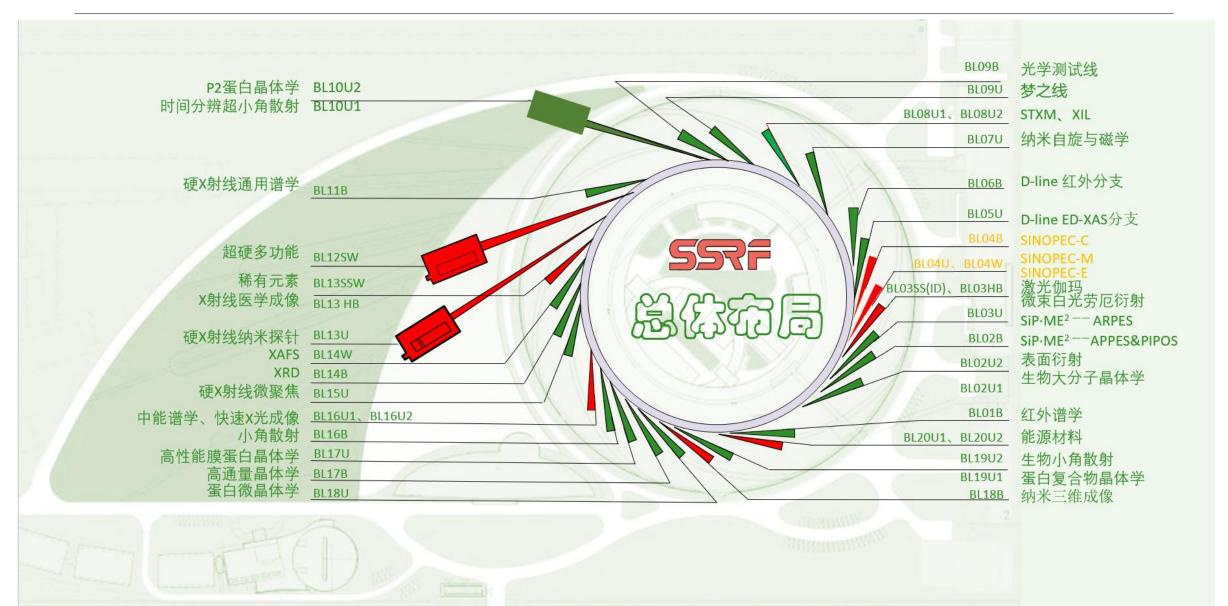
Current: 200~300mA (Top up)

**Emittence:** 4.2 nm-rad

Life time: ~ 20 hrs

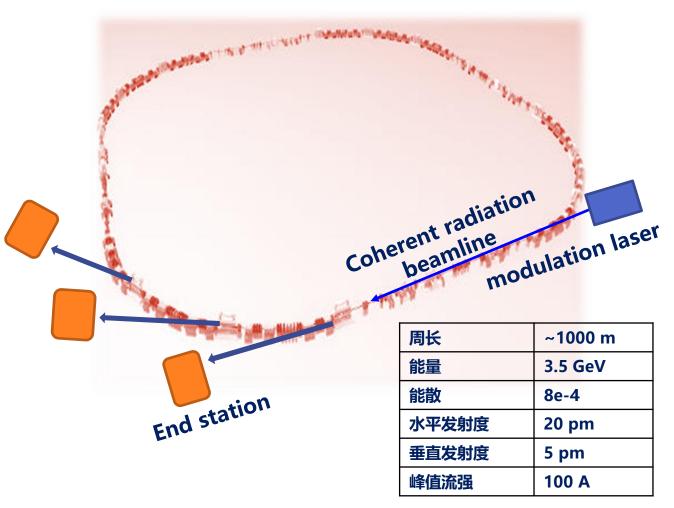


#### 34 beamlines with 46 end stations in operation



#### Design of the new generation synchrotron radiation source in Shanghai





	4th	5th
repetition frequency	100~500MHz	1~100MHz
Orbital stability	亚微米	亚微米
radiation stability	<1%	~1%
energy resolution	~100 meV	~0.1meV
time resolution	~10ps	0.1fs~10ps
average brightness	~10 <sup>22</sup>	<b>&gt;10</b> <sup>24</sup>
Coherent photon flux	~10 <sup>12</sup>	<b>&gt;10</b> <sup>14</sup>

The new generation of light sources combines the advantages of synchrotron radiation and free electron lasers to form a fully coherent light source with higher brightness and flux, wider pulse width regulation range, stable orbit and radiation, and richer experimental methods

