

Chapt 6 X-rays

- 6.1. Discovery of X-rays & their wave nature
- 6.2. Mechanisms for producing X-rays
- 6.3. Compton scattering
- 6.4. Absorption of X-rays
- 6.5 . Summary

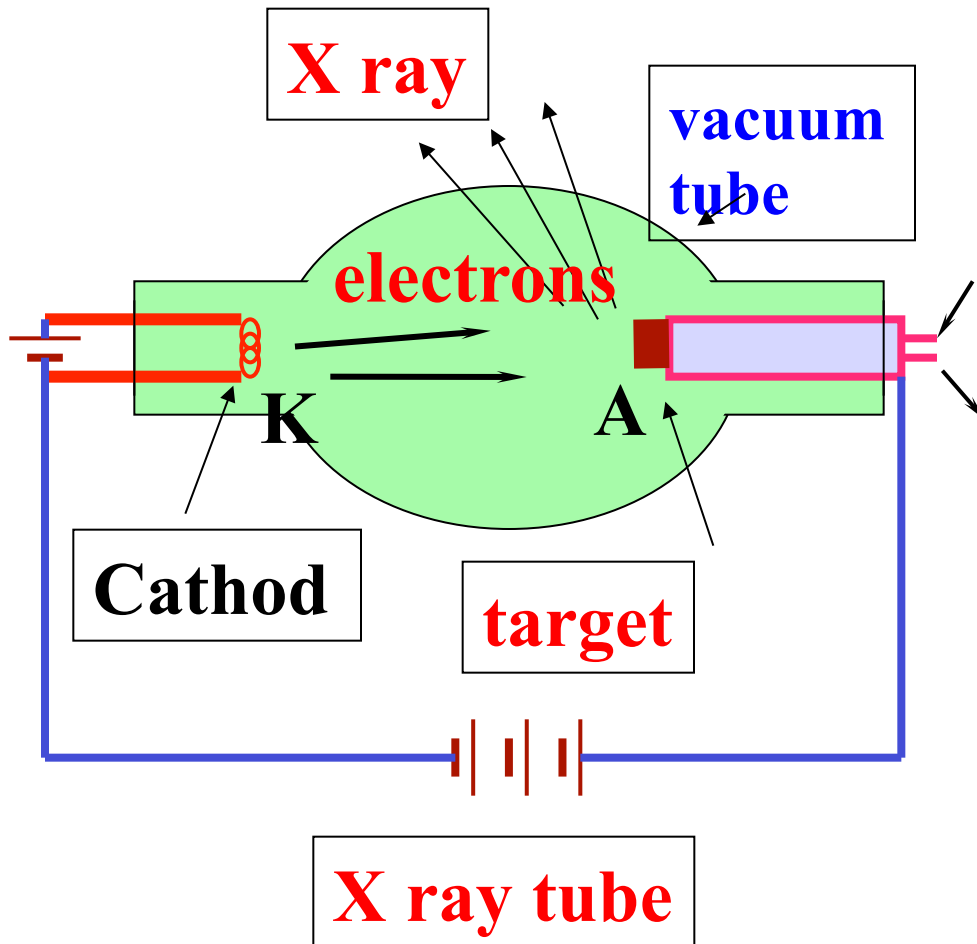
6.1. Discovery of X-rays & their wave nature

6.1.1. Discovery of X-rays

- **In 1895 , Roentgen performed an experim.on a gas discharge in a cathode ray tube in a darkroom, found a fluorescent screen exhibited slight fluorescence by a mysterious new rays:**
 - **Traveled straight**
 - **Strong penetrating power (neither reflection nor refraction)**
 - **Not deflected by a Magnetic field**
 - ***x -rays***

- **People realized that:**
 - **x-rays are energetic em wave with strong penetrating power**
 - **X-rays are EM wave with short wave length**
(L) : **0.001nm — 1 nm**
 - **Soft x ray: $L > 0.1\text{nm}$**
 - **Hard x rays: $L < 0.1\text{nm}$**

6. 1. 2. X-ray tube (1)



electrons from heated K are accelerated by E and strike on the Anode , producing x-rays

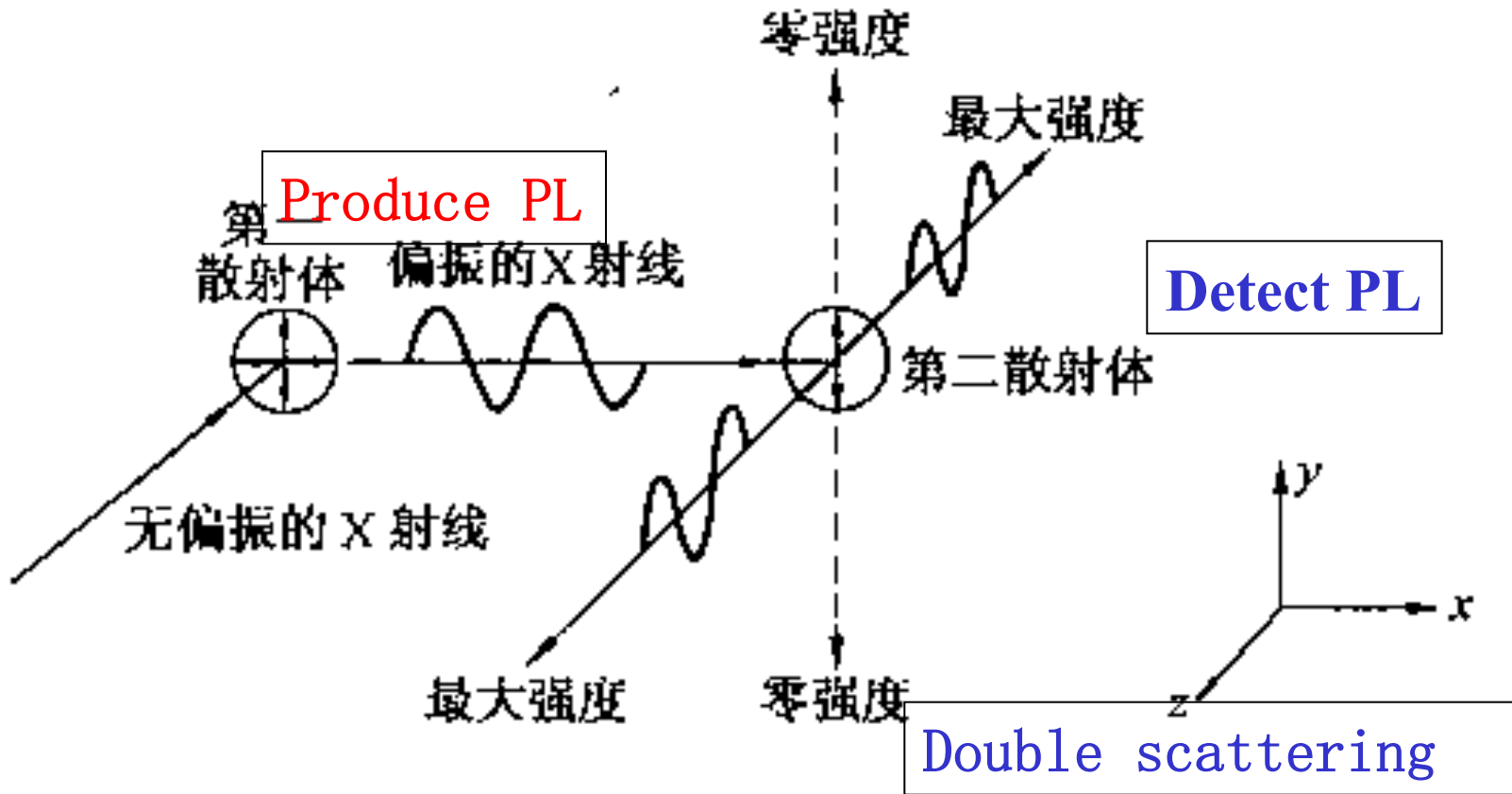
6.1.3. Wave nature of X-rays

- Accelerating charged particles \rightarrow radiate EM waves
- In x-ray tube, high speed Es stop on the Anode \rightarrow radiate EM waves
- X-rays \leftrightarrow EM waves
- Characters of wave
 - polarization, diffraction

6.1.4 Polarization of X-rays

- Transverse wave: oscillating direction is perpendicular to the propagation direction
 - EM wave is transverse wave (E, K)
 - PL concept only holds for transverse wave
- **Linear PL:** *E oscillates along a fixed direction*
- **Circular PL:** *E moves along a circle*

Double scattering experiment



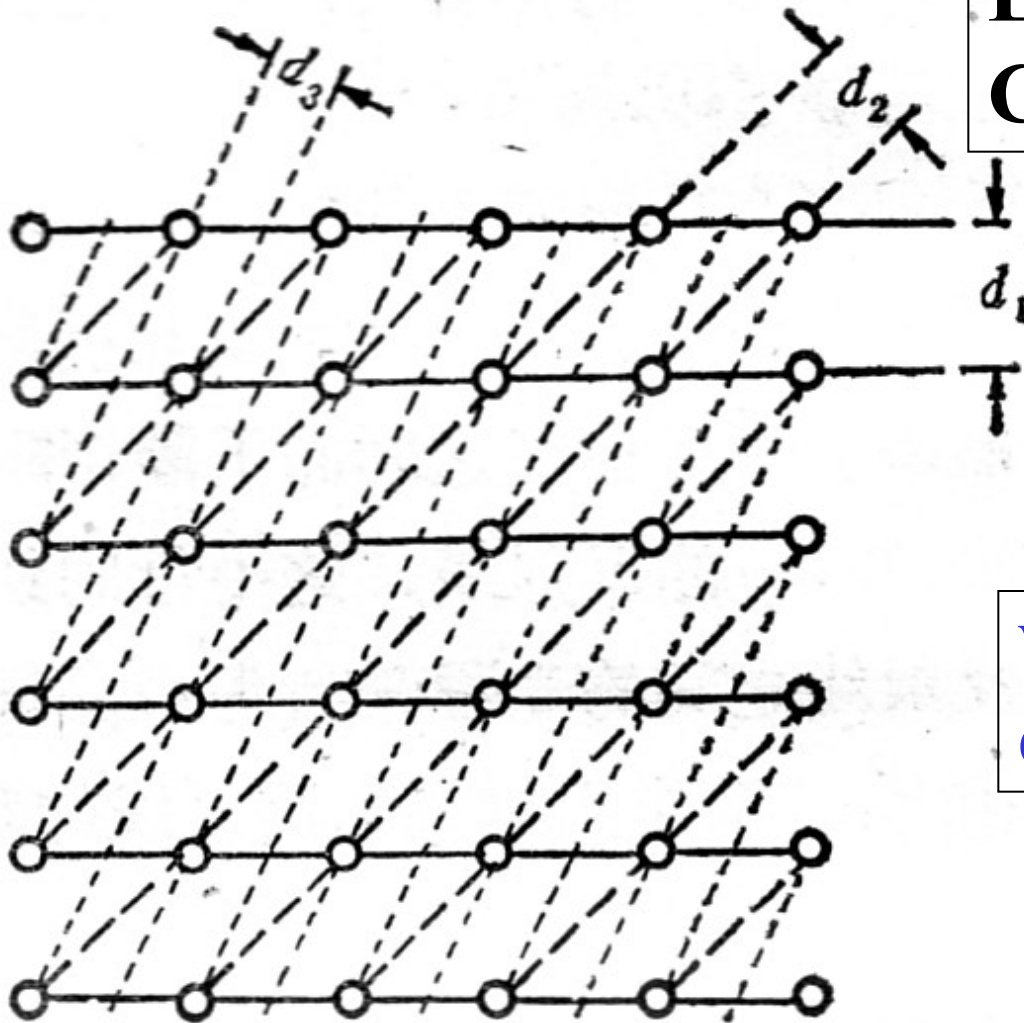
unPL waves strike on the 1st scatterer in z perpend. to xy-plan , producing y-PL wave in x direction ; after 2nd scattering, one observes y-PL waves in the z -, but not in the y- direction.

6.1.5. Diffraction of X-rays

- EM wave passes through a slit → diffraction
(Slit size is the same order as Wavelength λ)
- Typical λ of x-rays : **0.1nm (hard to build slit)**
- **crystal: atoms (lattice) in ordered -structure**
 - **晶格常数 d : crystal lattice distance is in the same order as λ of x-rays**
- crystal is a natural grating (set of slits)

Crystal planes

**Lattices form many
Crystal planes**

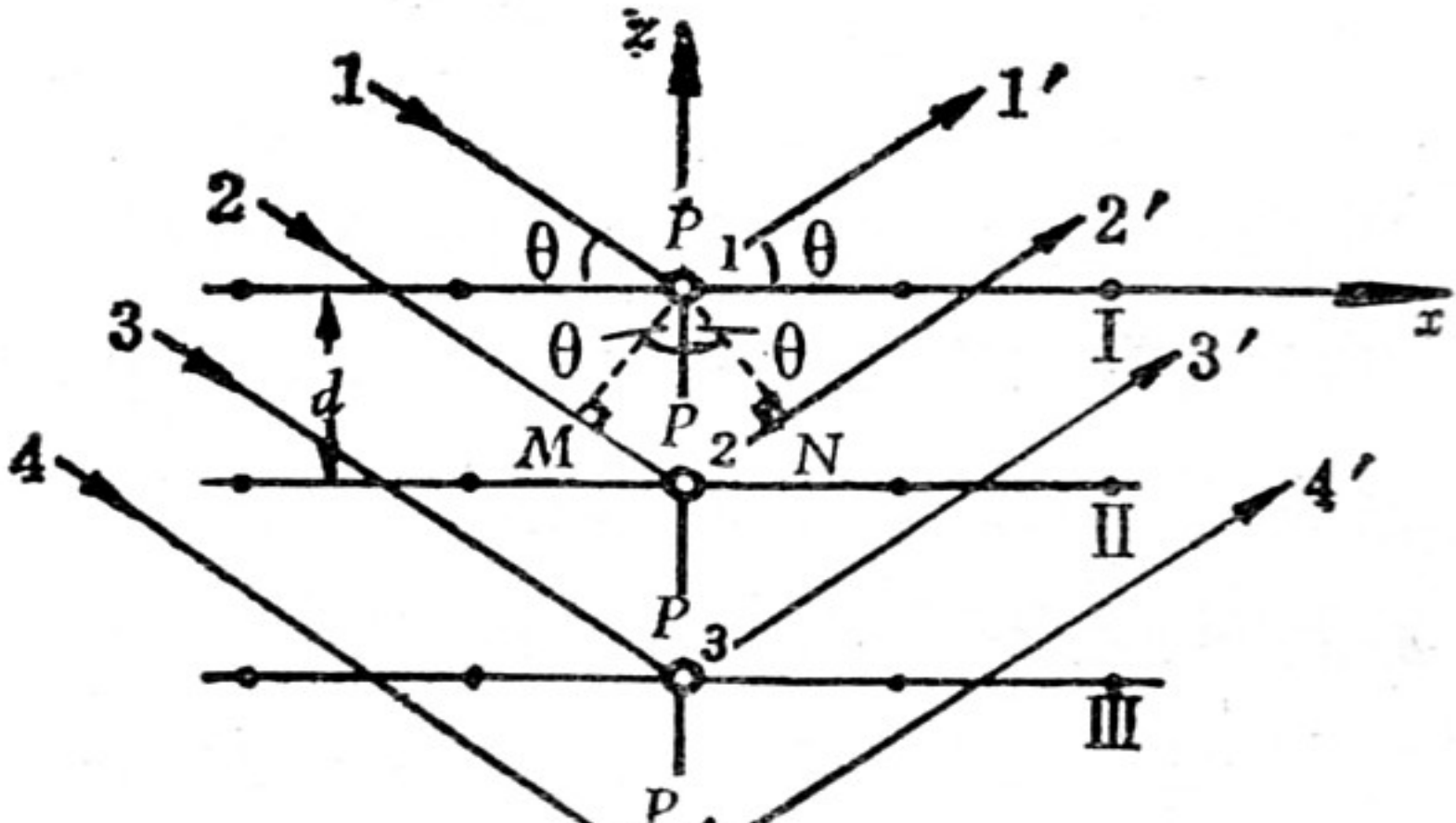


**With different lattice
distances**

Interference btw parallel planes

Path difference btw ray 1 & ray 2

$$\delta = \overline{MP_2} + \overline{P_2N} = d \sin \theta + d \sin \theta = 2d \sin \theta$$



Bragg Law

When the path difference is an integral of λ ,
there exists a maximum in diffraction intensity

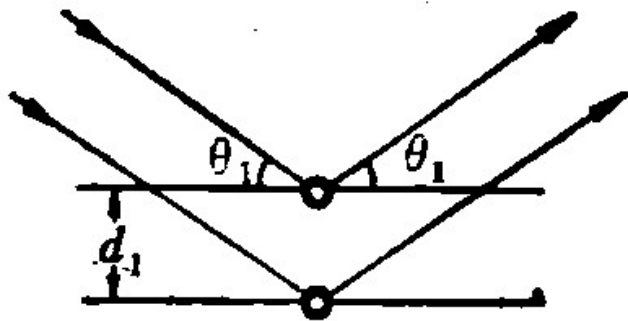
$$2d \sin \theta = n\lambda \quad (n = 1, 2, 3, \dots)$$



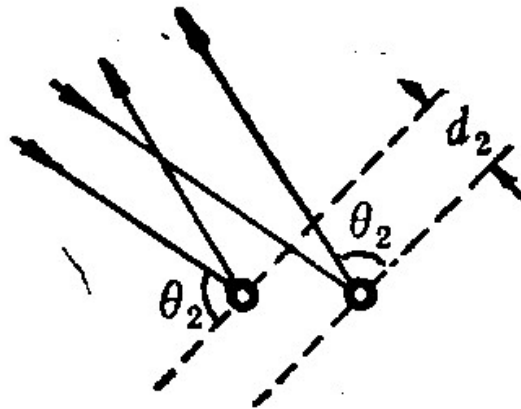
Bragg formula

- Giving incident direction of X-ray, WL λ and cristal \rightarrow a set of Bragg equations
 - Many sets of crystal planes
 - One set of crystal palne \rightarrow one Bragg Equation

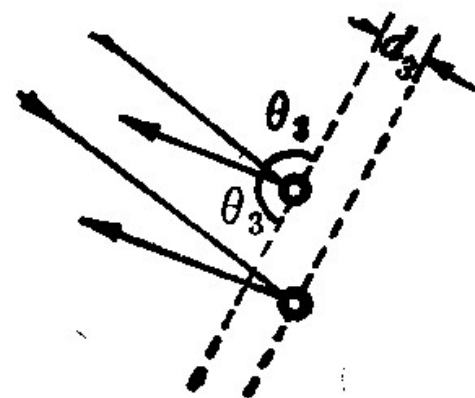
$$2d_1 \sin \theta_1 = n_1 \lambda$$



$$2d_2 \sin \theta_2 = n_2 \lambda$$



$$2d_3 \sin \theta_3 = n_3 \lambda$$



Application of X-ray diffraction

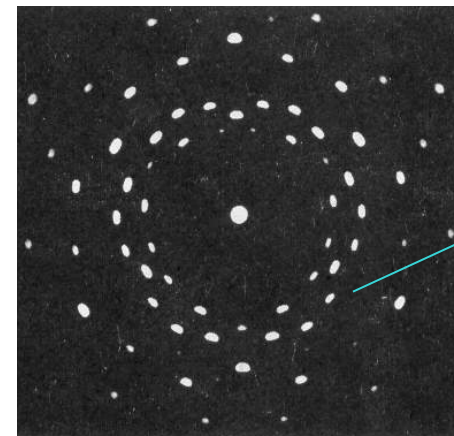
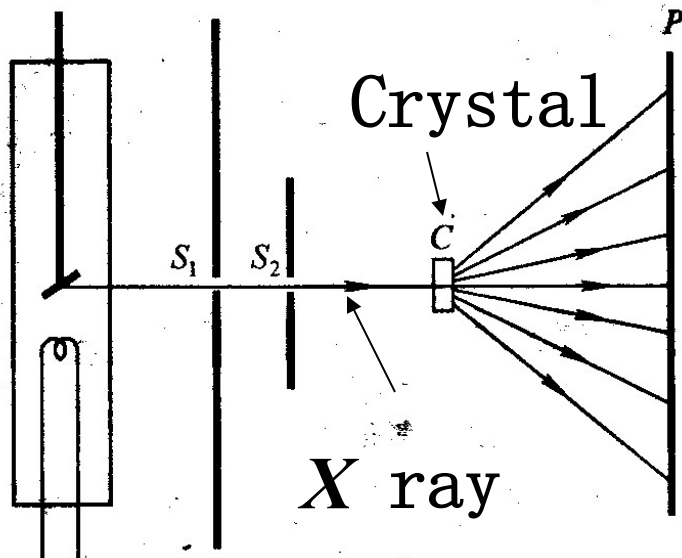
- Giving θ, λ , one can measure d — study crystal structure and properties,
- Giving θ, d , one can measure λ — using X ray light spectra, to study
- Atoms structure

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

Methods to observe x-ray diffraction

- Laue film method

- Using continuous WL X-ray to a single crystal
- Giving direction, arbitrary WL
- Each set of crystal planes, satisfy $2d \sin \theta = n\lambda$
- Gives a Laue spot, the position stands for the direction of the related planes → obtain all maximums. Each maximum has a bright spot

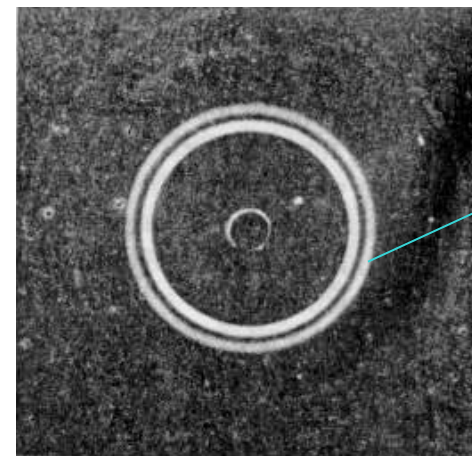
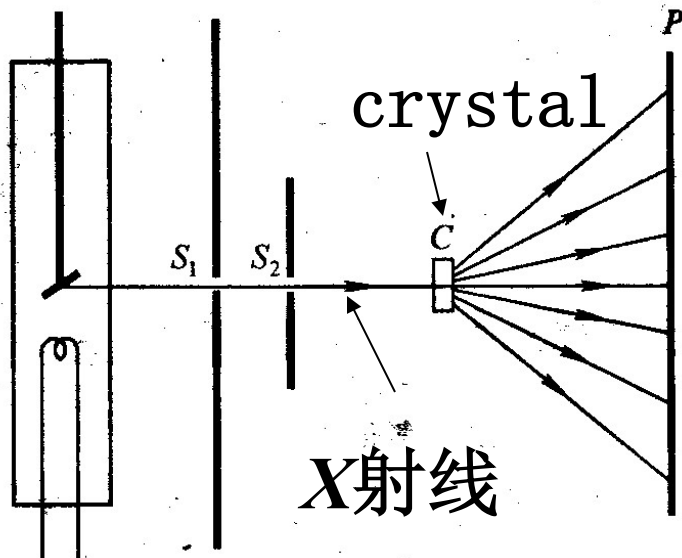


- Polycrystalline powder method

- Using fixed WL x ray on polycrystalline powder , the planes directions are arbitrary

- , the set of planes satisfying $2d \sin \theta = n\lambda$ gives a con-centric circle

- \rightarrow many circles \leftrightarrow many set of planes



Measured

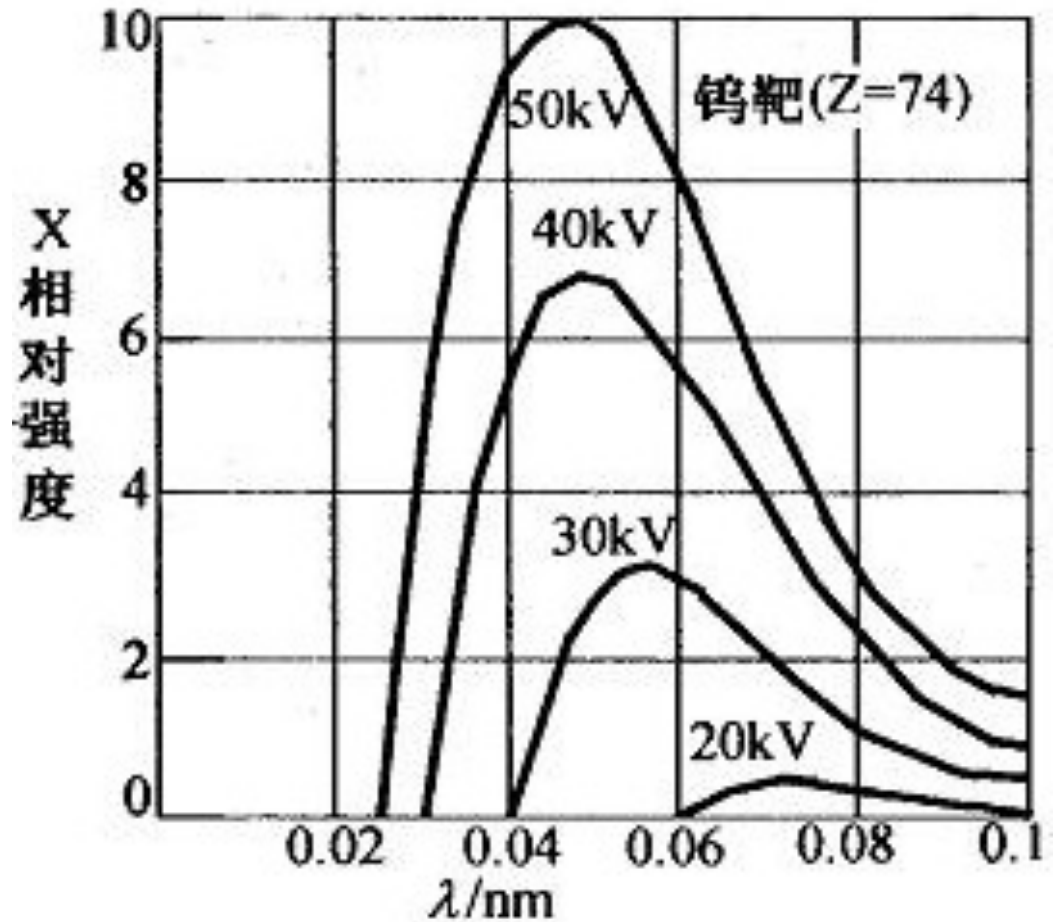
6. 2. Mechanisms for producing X-rays

6.2.1. X-ray emission spectra

X-ray emission intensity versus Wavelength

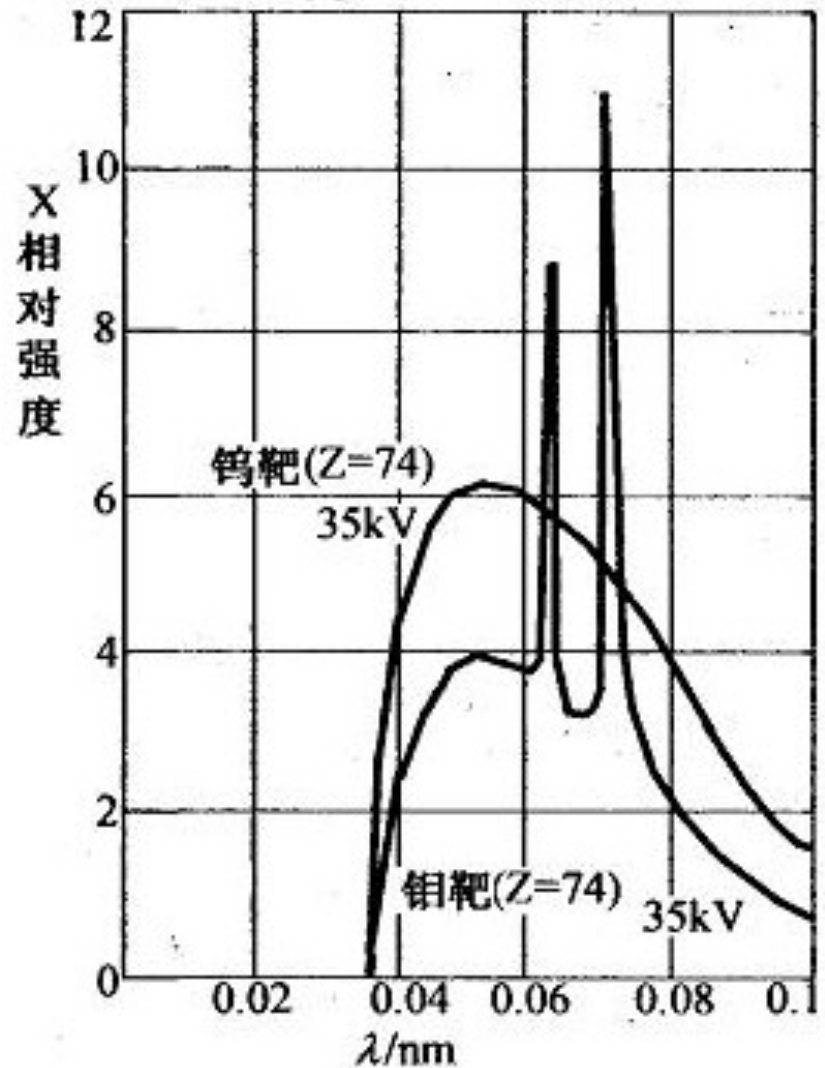
Continuous spectra:

The minimum WL depends
On applied potential



Characteristic spectra

Peaks depend on target



6. 2. 2. Cont. Spectra--Bremsstrahlung

- **Bremsstrahlung**
 - Charged particles in acceleration produce EM waves
- **Continuous spectra**
 - **X-ray tube**, charged Es reach the target, their speed changes continuously under the Coulomb field of the target atoms, induce cont. x-ray spectra
- **The minimum WL depends on V**
- **X-ray emission due to de-acceleration**

- λ_{\min} ,depends only on applied voltage V :
 - Obtained kinetic energy eV transfers to the energy of emission photons, λ_{\min}

$$eV = h\nu_{\max} = h \frac{c}{\lambda_{\min}} \rightarrow \lambda_{\min} = \frac{hc}{e} \cdot \frac{1}{V} = \frac{1.24}{V(\text{kV})} \text{ nm}$$

↓
 planck h

↓
 Agrees with data

λ_{\min} confirms once more the success of quantum theory

6. 2. 3. Character spectra—transitions of the inner shell electrons

- **Threshold energy or ionization energy:**
for removing one e from $n=1$ shell
- K_{α} spectra energy : energy difference from $n=2$ and $n=1$
- Atomic light spectra is determined by the
- External electrons , their configuration's periodic behavior leads to its periodic
- K_{α} spectra determined by transitions in inner shells

- Giving elements, charat. spectra contain several series
 - **K series spectra**: $K_{\alpha}, K_{\beta}, K_{\gamma}, \dots$,
 - **L series spectra**: $L_{\alpha}, L_{\beta}, L_{\gamma}, \dots$,
 - **M series**: $M_{\alpha}, M_{\beta}, M_{\gamma}, \dots$,
 - **N series**: $N_{\alpha}, N_{\beta}, N_{\gamma}, \dots$,
- K_{α} spectra frequency Moseley formula

$$\nu_{K_{\alpha}} = 0.246 \times 10^{16} (Z - \sigma_K)^2 \text{ Hz}$$

$$\sigma_K \approx 1$$

Provides a precise measuring method of Z

Interpret Moseley formula

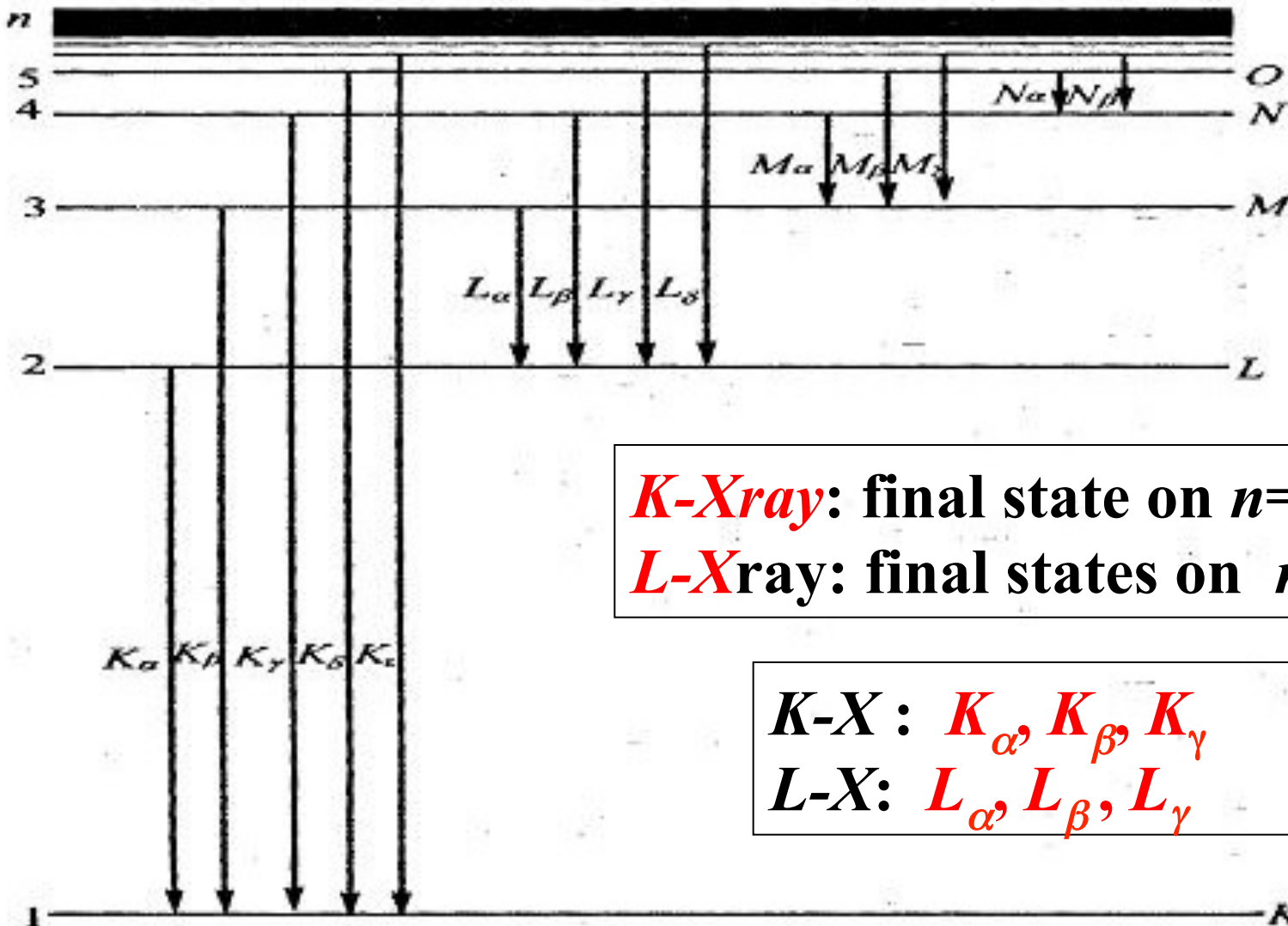
- when $n=1$ shell has a vacancy, Es in $n=2$ shell sense the attraction of positive charges of $(Z-1)$, and transit to the inner shell, producing K_α
- $(n=2 \rightarrow n=1)$ transition $\rightarrow K_\alpha$ spectra freq.

$$\begin{aligned} \nu_{K_\alpha} &= \frac{c}{\lambda} = Rc \left(\frac{1}{1^2} - \frac{1}{2^2} \right) (Z-1)^2 = \frac{3}{4} Rc (Z-1)^2 = \frac{3}{4} \frac{13.6}{h} (Z-1)^2 \\ &= 0.248 \times 10^{16} (Z-1)^2 \end{aligned}$$

Agrees with Moseley

Transition e fell attraction from-
(z-1) positive charge

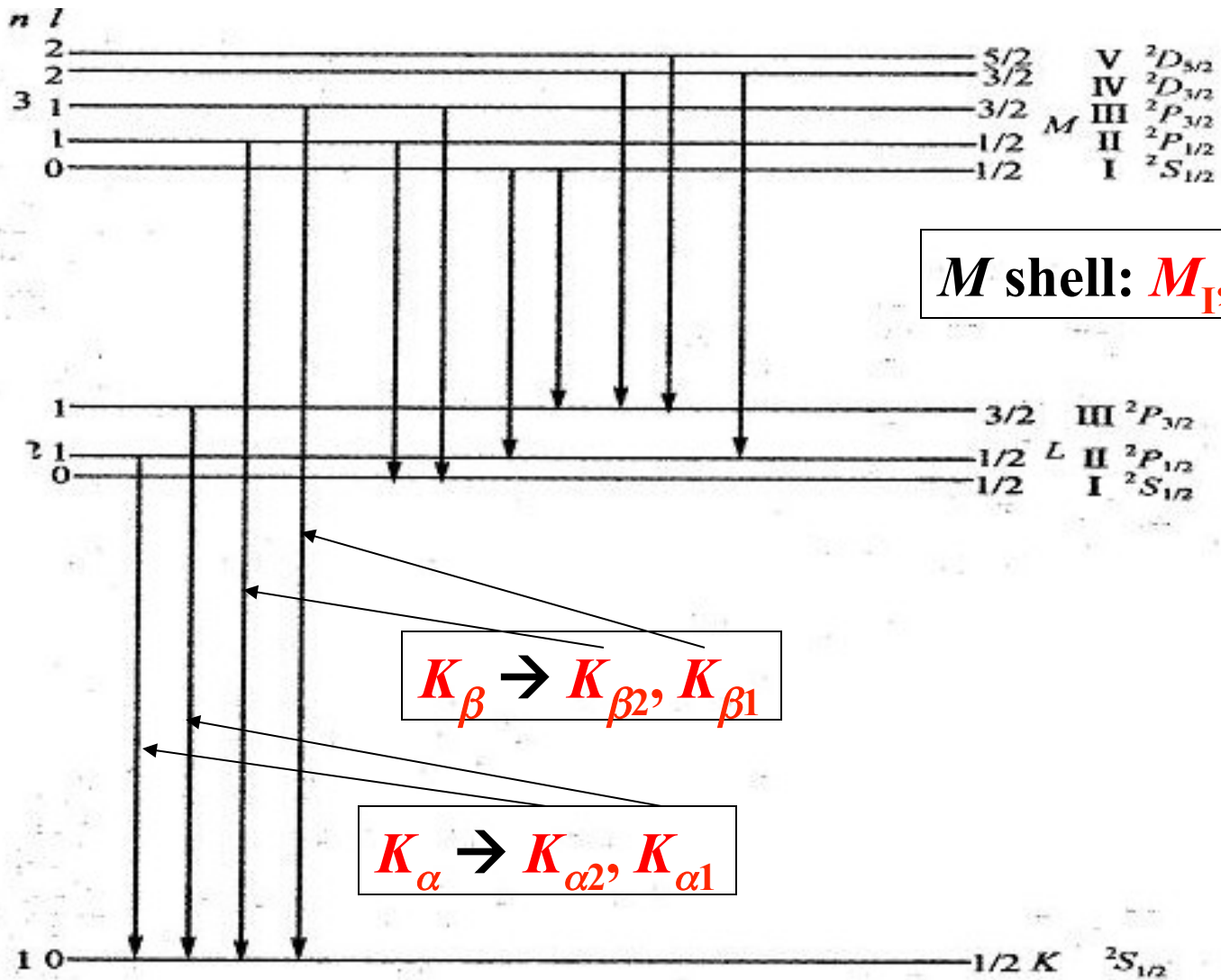
6. 2. 4. labeling of the charact. X-ray



K-Xray: final state on $n=1(K)$ shell
L-Xray: final states on $n=2(L)$ shell

K-X : $K_\alpha, K_\beta, K_\gamma$
L-X : $L_\alpha, L_\beta, L_\gamma$

With fine structure



M shell: $M_I, M_{II}, M_{III}, M_{IV}, M_V$

L shell: L_I, L_{II}, L_{III}

$K_\beta \rightarrow K_{\beta 2}, K_{\beta 1}$

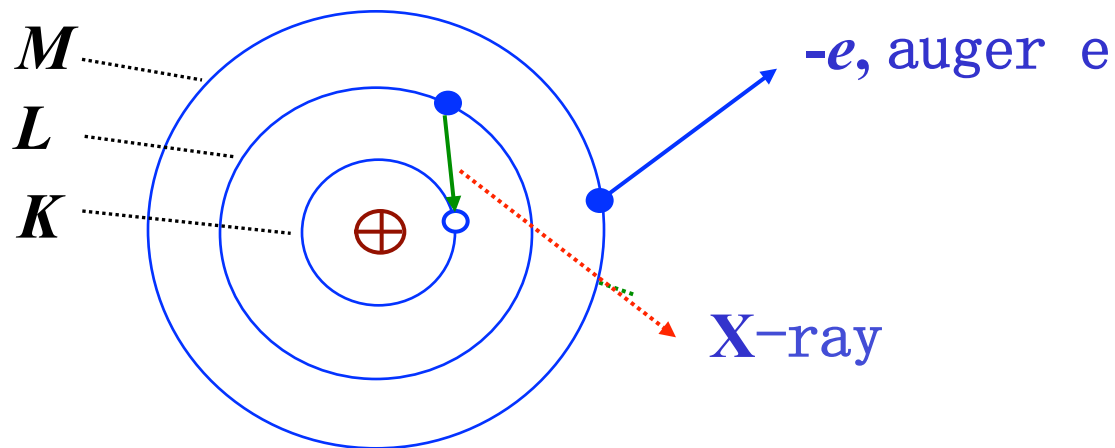
$K_\alpha \rightarrow K_{\alpha 2}, K_{\alpha 1}$

$$\Delta L = \pm 1;$$

$$\Delta J = 0, \pm 1$$

6. 2. 5. Auger Electrons

- An external shell e transits to a vacancy, without **X-ray radiation**, transfers its energy to another e in the same shell or outer-shell, and makes it escape from the atom



Kinetic energy : $(\phi_K - \phi_L) - \phi_M$

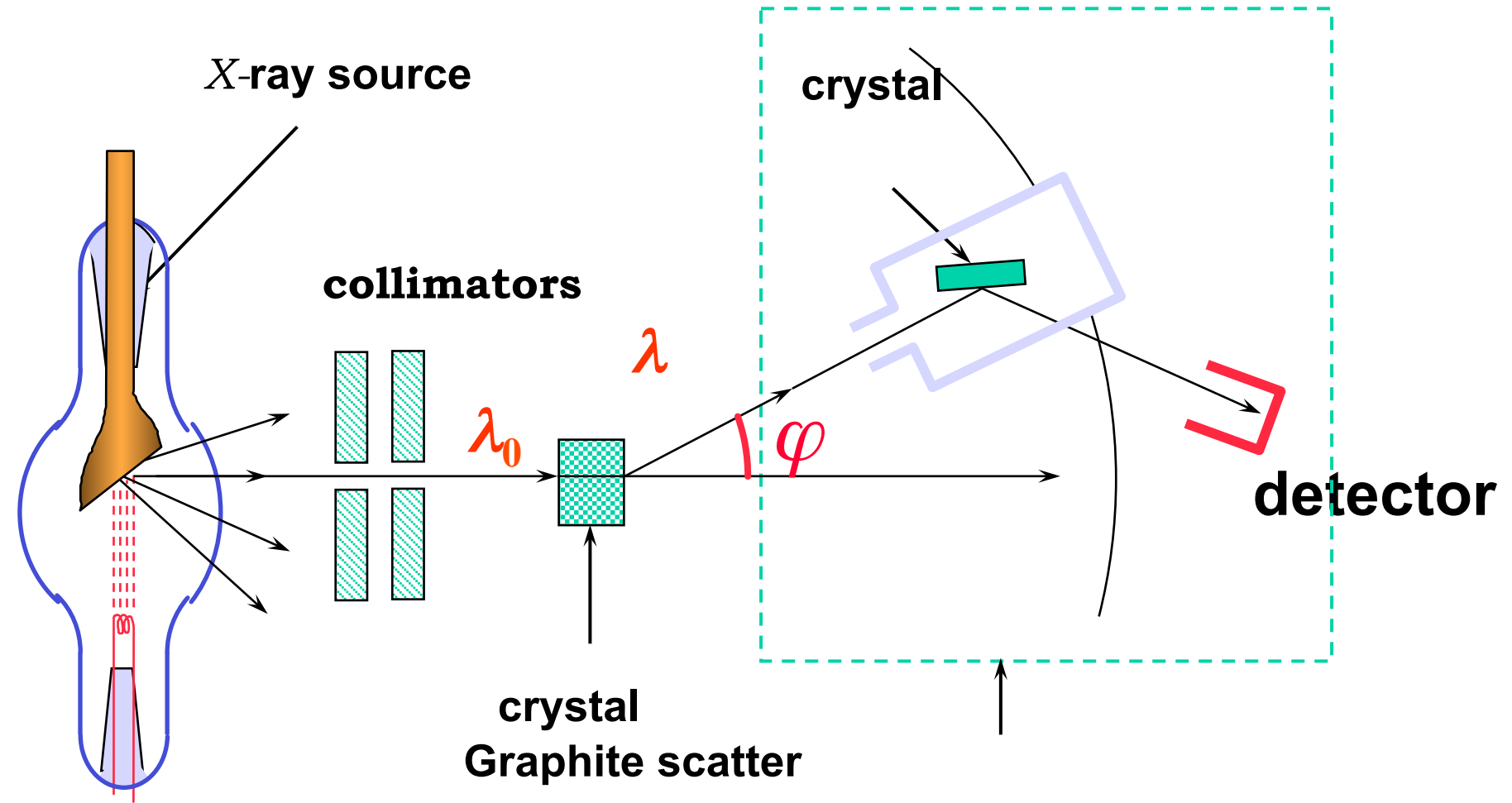
6. 2. 6. Synchrotron Radiation

- **The radiation produced by es moving in a circular paths in a sychrotron accelarator .**
 - A new type of powerful *X-ray*
- **properties:**
 - **Width of enegy spectra $0.1 \sim 10^4 \text{ \AA}$**
(continuous)
 - **Big power : 10 kW; X-ray tube :10 W**
 - **Highly polarized**
 - **Well-collimated in direction**

6. 3. Compton Scattering

- In 1923, Compton proved the particle nature of x-ray in an experiment by scattering x-ray on matter

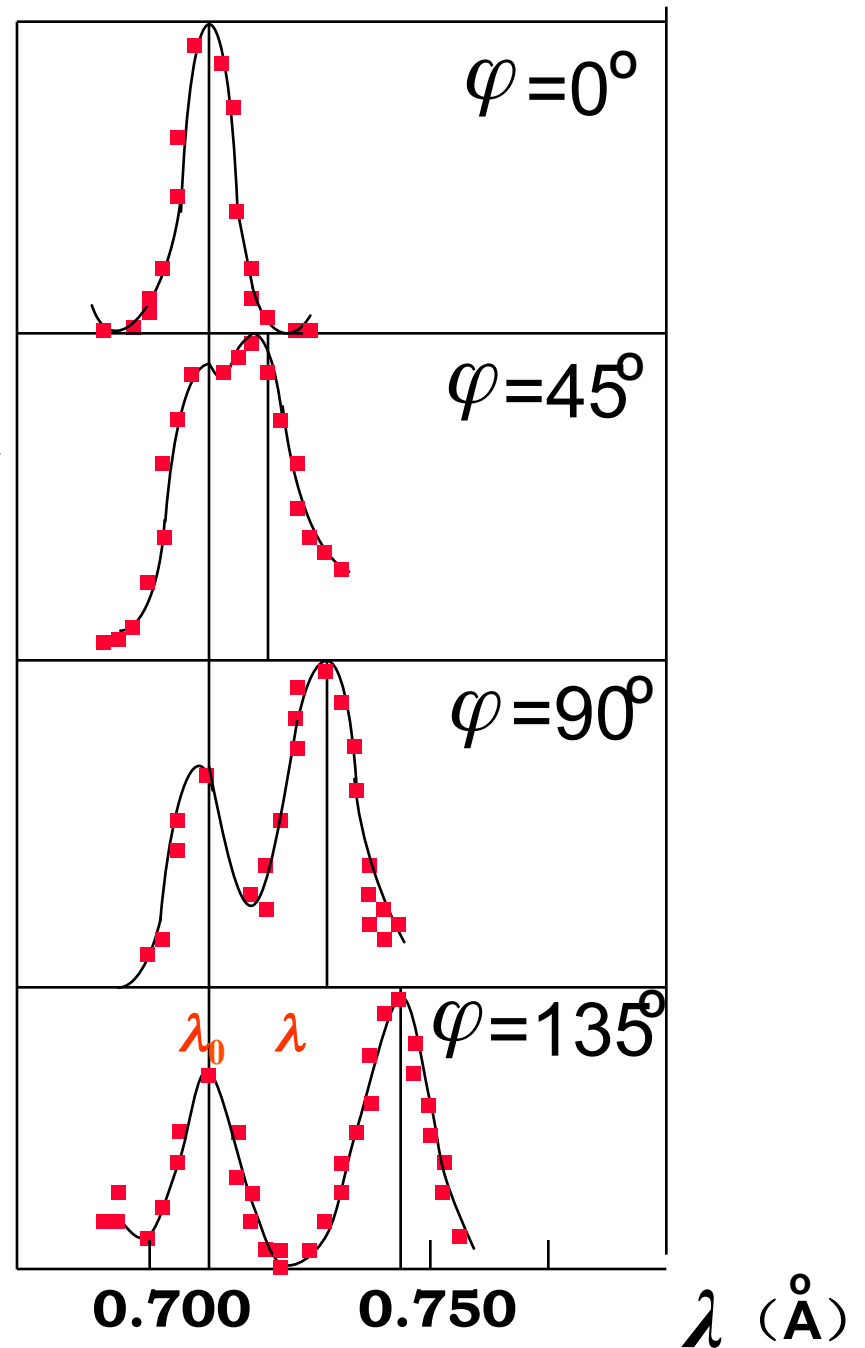
6.3.1. compton scattering exp



6.3.2. scatter curves

Experiment curve

Scattered x-ray has
Original and longer
wavelenths



Three Characters of the scattering curves

- Besides original λ_0 , there appear new bigger λ

$$\Delta\lambda = \lambda - \lambda_0$$

- The increase of WL, depends only on φ , not on scatters and λ_0

$$\Delta\lambda = \lambda - \lambda_0 = \lambda_c (1 - \cos \varphi)$$

$$\lambda_c = 0.0241 \text{ \AA} = 2.41 \times 10^{-3} \text{ nm}$$

- With increase scattering angle, the intensity of original λ_0 decreased, while that of the new WL increases

6.3.3. Classical consideration

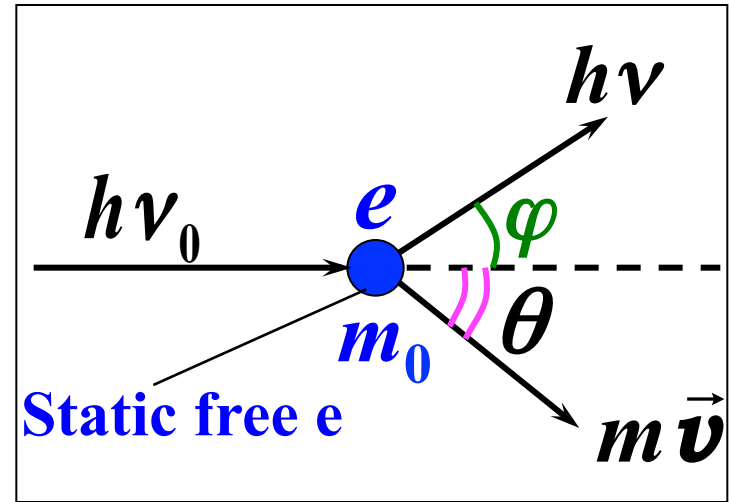
- **Classical EW theory:** when a EW passes through material, the scattered EM should have the same WL as the incident one
 - incident X ray exerts on the Es in atoms
 - Es oscillate with the same freq. as the incident wave

fails to explain compton scattering

6.3.4. Quantum Explanation

- *X rays scatter on static external Es*
 - X-ray energy $\epsilon \sim 10^4 \text{ eV}$
 - The bounding energy of external $E_s \sim \text{eV}$
 - can be treated as free E_s
- **Elastic scattering**
 - Energy and momentum conservation
 - Photon transfers part of its energy to electron, decreases its energy and hence increases its WL

- E & P conservation



$$h\nu_0 + m_0c^2 = h\nu + mc^2$$

$$\frac{h}{\lambda_0} \vec{n}_0 = \frac{h}{\lambda} \vec{n} + m \vec{v}$$

$$mc^2 = m_0c^2 + h(\nu_0 - \nu) = m_0c^2 + hc\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right)$$

$$(mc^2)^2 = (m_0c^2)^2 + 2m_0c^3h\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) + (hc)^2\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right)^2$$

$$(m v)^2 = \left(\frac{h}{\lambda_0}\right)^2 + \left(\frac{h}{\lambda}\right)^2 - 2\frac{h^2}{\lambda_0\lambda} \cos \varphi$$

$$(mc^2)^2 = (m_0c^2)^2 + 2m_0c^3h\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) + (hc)^2\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right)^2$$

$$(mv)^2 = \left(\frac{h}{\lambda_0}\right)^2 + \left(\frac{h}{\lambda}\right)^2 - 2\frac{h^2}{\lambda_0\lambda}\cos\varphi$$

$(-)\times c^2$

$$\cancel{(mc^2)^2}\left(1 - \frac{v^2}{c^2}\right) = \cancel{(m_0c^2)^2} - 2(hc)^2\frac{1}{\lambda_0\lambda} + 2\frac{h^2c^2}{\lambda_0\lambda}\cos\varphi + 2m_0c^3h\frac{\Delta\lambda}{\lambda_0\lambda}$$

$$\rightarrow \frac{m_0c}{h}\Delta\lambda = 1 - \cos\varphi$$

$$\Delta\lambda = \lambda_c(1 - \cos\varphi)$$

Compton formula

$$\lambda_c = \frac{h}{m_0c} = \frac{hc}{m_0c^2} = \frac{1.24}{511} = 0.00243\text{nm}$$

Agrees with data

Energy of scattered photon

$$\lambda - \lambda_0 = \lambda_c (1 - \cos \varphi) \longrightarrow \frac{1}{h\nu} - \frac{1}{h\nu_0} = \frac{1}{m_0 c^2} (1 - \cos \varphi)$$

$$\boxed{* (hc)^{-1}}$$

$$\rightarrow h\nu = \frac{1}{\frac{1}{h\nu_0} + \frac{1 - \cos \varphi}{m_0 c^2}} = \frac{h\nu_0}{1 + \frac{h\nu_0}{m_0 c^2} (1 - \cos \varphi)} = \frac{h\nu_0}{1 + \gamma (1 - \cos \varphi)}$$

$$\gamma = \frac{h\nu_0}{m_0 c^2} = \frac{hc}{m_0 c^2 \lambda_0} = \frac{\lambda_c}{\lambda_0}$$

Kinetic E of the recoiling electrons

$$h\nu_0 + m_0c^2 = h\nu + mc^2$$

$$\begin{aligned}\rightarrow E_r &= mc^2 - mc_0^2 = h\nu_0 - h\nu \\ &= h\nu_0 \frac{\gamma(1 - \cos\varphi)}{1 + \gamma(1 - \cos\varphi)}\end{aligned}$$

6.3.5. The physical meaning

- Compton WL of the electron

$$\lambda_c = \frac{h}{m_0 c} = \frac{hc}{m_0 c^2} = \frac{1.24}{511} = 0.00243 \text{ nm}$$

- **When the E of incident photon equals the rest E of the electron**

$$h\nu_0 = m_0 c^2 \rightarrow h \frac{c}{\lambda_0} = m_0 c^2 \rightarrow \lambda_0 = \lambda_c = \frac{h}{m_0 c}$$

- **When $\varphi = 90^\circ$, the WL difference of incident and scattered waves**

$$\Delta\lambda = \lambda_c (1 - \cos\varphi) \rightarrow \varphi = 90^\circ, \quad \Delta\lambda = \lambda_c = \frac{h}{m_0 c}$$

Reduced Compton WL

$$\lambda'_c = \frac{h}{m_0 c} = \frac{4\pi\epsilon_0 hc}{e^2} \cdot \frac{e^2}{4\pi\epsilon_0 m_0 c^2} = \frac{r_e}{\alpha}; 137r_e$$

– **Classical radius of the electron**

$$m_0 c^2 = \frac{e^2}{4\pi\epsilon_0 r_e} \rightarrow r_e = \frac{e^2}{4\pi\epsilon_0 m_0 c^2}; 2.8\text{fm}$$

RCWL is 137 times of r_e

Some discussions

- Why $\Delta\lambda$ is independent of scattered material ?
 - Free electrons
- Why some of the scattered rays have its original WL?

$$m_{\text{原子}} \gg m_{\text{光子}}$$

- Coherence : $\Delta\lambda=0$
- Non-coherence : compton scattering

- Why there is no WL shift w/ visible light scattering?

$\Delta\lambda$ does not depend on λ_0 , only on φ ; $\varphi=180$,
the maximum of $\Delta\lambda = 0.0049\text{nm}$; visible light
 with $\lambda_0 \sim 500\text{nm}$; $\rightarrow \Delta\lambda/\lambda_0$ is too small

- Why the free electrons do not absorb, but scatter photons?
 - If it do absorb photon

$$h\nu_0 + m_0c^2 = mc^2 \quad m = m_0 / \sqrt{1 - v^2/c^2}$$

$$\frac{h\nu_0}{c} \hat{n}_0 = m v \hat{n}_0 \quad \Rightarrow 1 - \frac{v}{c} = \sqrt{1 - \frac{v^2}{c^2}}, \Rightarrow v = c$$

Significances of Comp. Scatter

- Provides strong supports for photon' s quanta hypothesis
- Proof of photon' s momentum
- Verified that **Energy-momentum conservation is still valid** in single event of microscopic world,

6.3.6. Comp. Scattering & fundamental constants

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

→ measure $\Delta\lambda$, φ , if one knows two of

h, m_0, c

One can measure the other one

- **Measure the energy of photon**

$$E_r = h\nu_0 \frac{\gamma(1 - \cos\varphi)}{1 + \gamma(1 - \cos\varphi)} \quad \gamma = \frac{\lambda_c}{\lambda_0}$$

→ measuring E_k , φ , λ_0 , one can obtain the energy of the incident photon

6.4. The Absorption of X-rays

- **Absorption rules**
- **Micro-mechanism of x-ray absorp.**
- **Absorption of x-ray**

6. 4. 1. Absorption rules of x-ray

- X-ray passes through material \rightarrow its intensity is reduced

- $x = 0, \quad I_0$

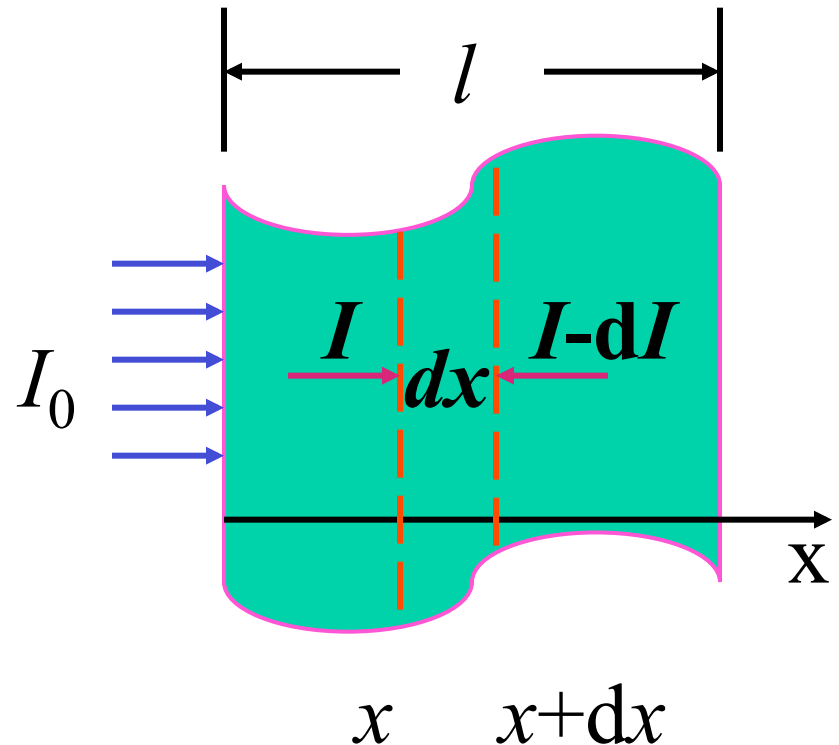
- $x = x, \quad I(x)$

- $x = x+dx, \quad I(x) - dI$

- $-dI = \propto dx I(x)$

- Absorption coefficient μ

- $\rightarrow -dI = \mu dx I(x)$



Integrate over (0 ~ x) → Lambert-Beer rule

$$I(x) = I_0 e^{-\mu x}$$

– **Absorption length: x** $x\mu = 1 \rightarrow x_0 = \mu^{-1}$

- After passing distance x_0 , the intensity is reduced by e^{-1}

– **Linear absorption coefficient : μ**

- x 's unite cm, μ ' s unite cm^{-1}

- **Absorbing matter density: ρ**

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

Mass thickness **mg / cm²**

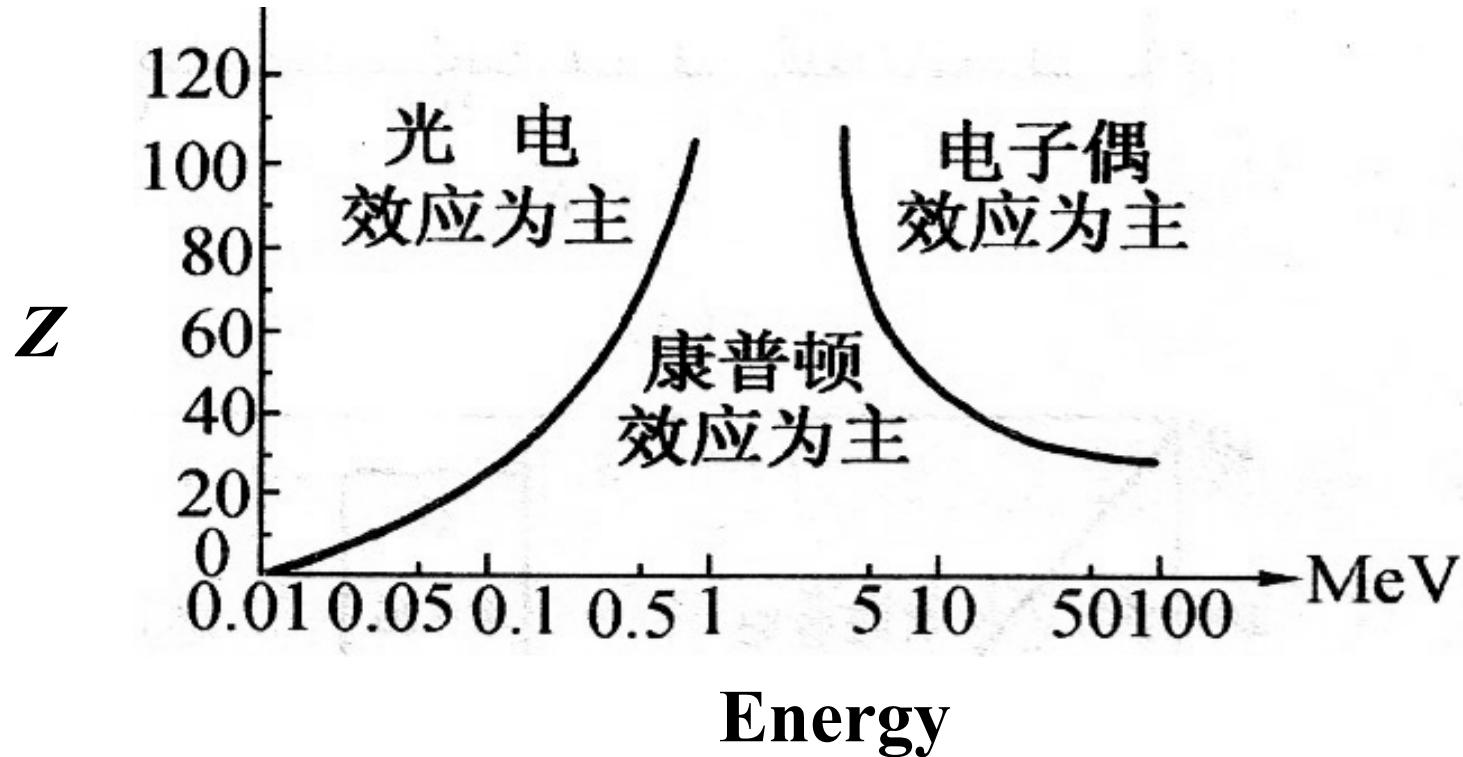
- **Mass absorption coefficient μ / ρ cm²/mg**
 - μ / ρ does not depend on the state of absorber (gas, liquid, solid)
- **Lambert-Beer rule**

$$I(x) = I_0 e^{-\frac{\mu}{\rho} x \rho}$$

6. 4. 2. Micro. Mechanism of x-ray absorption

- **Photoelectric effect**
 - Photons interact with bound electrons , being completely absorbed
- **Compton effect**
 - Photons scatter with free electrons (external shell)
- **Pair production**
 - When photon energy is larger than $2m_0$ (1.02MeV), photon splits into e^-e^+ pair

Relative importance of 3 major interactions btw photons and matter



$$I(x) = I_0 e^{-\frac{\mu}{\rho} x \rho} \quad \rightarrow \quad \mu = \mu_{\text{光电}} + \mu_{\text{康}} + \mu_{\text{相干}}$$

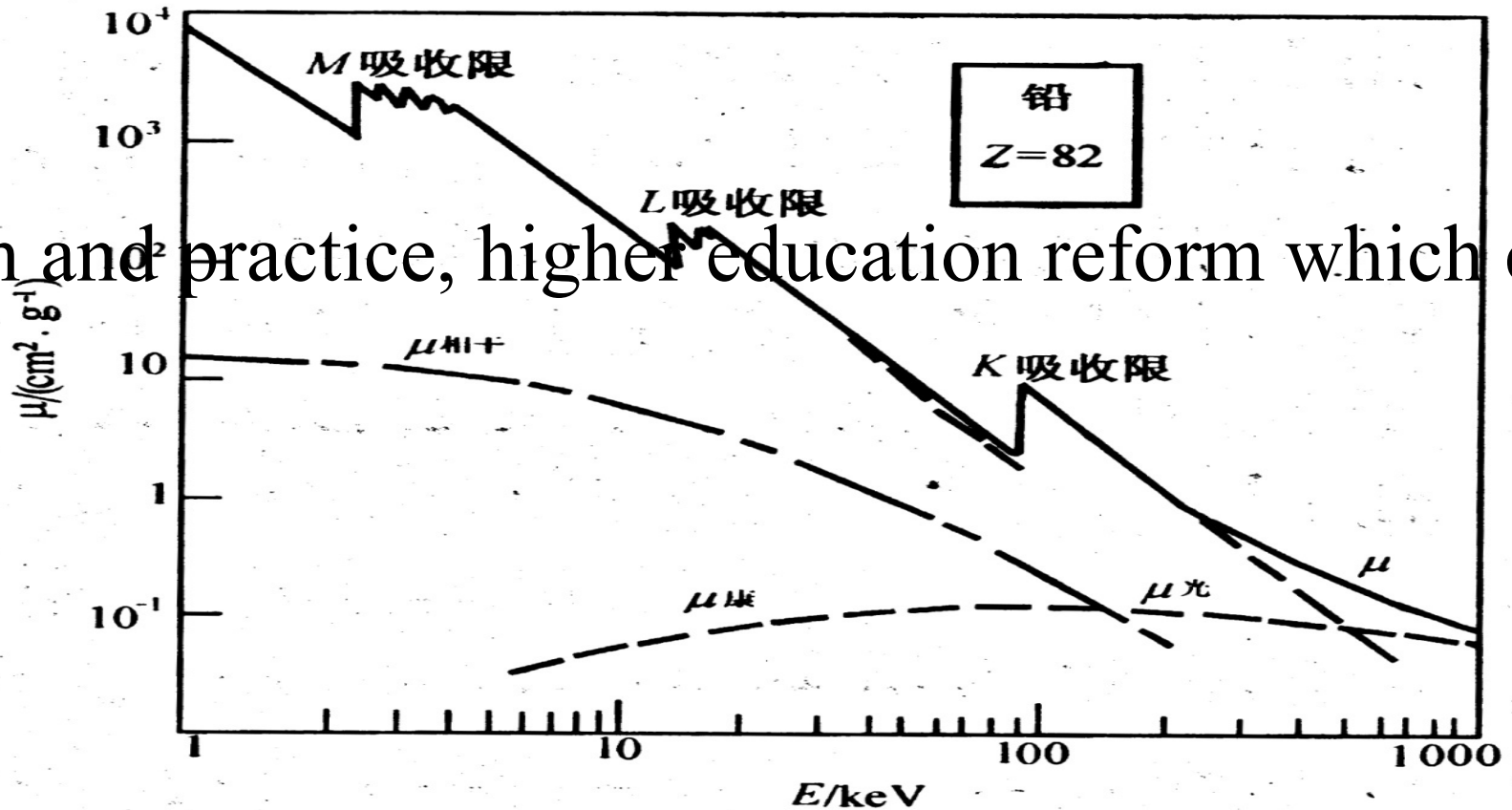
6.4.3 Absorption of x-ray

- **Matter with mixed elements**

$$\mu = \sum_j w_j \mu_j$$

- μ_j the absorption coefficient for j element
- w_j the ratios of j element in the matter
 $\sum_j w_j = 1$

Mass absorption coefficient versus incident energy



Decreasing with the increase of incident energy

Absorption edges

Peaks for sudden changing
Of μ , corresponding to
K、*L*、*M*...**absorption lines**
From energetic x photon
Removing *K*、*L*、*M* electrons
Thus induces resonance absorption

