Midterm Solution

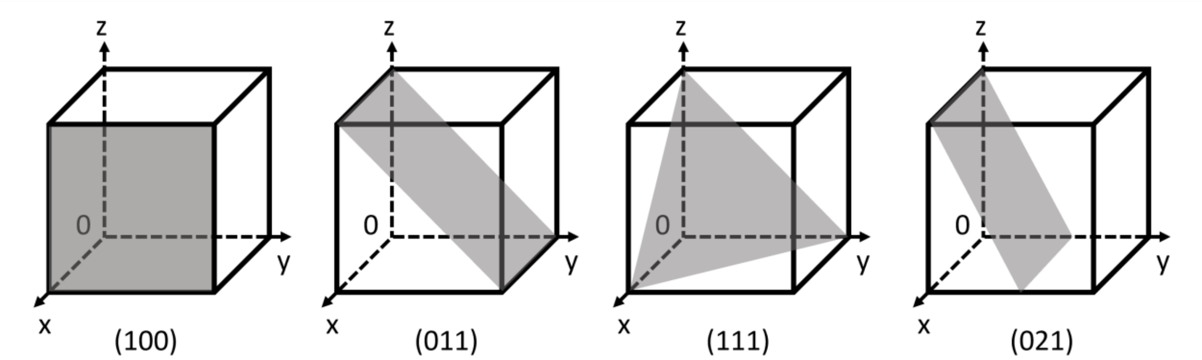
1. (1) When the X-ray tube voltage is higher than a critical value U_K of the target, a series of linear spectra with very high intensity and narrow wavelength range will appear at certain specific wavelength positions, called characteristic spectra.

(2) There will be vacancies after the incident electrons knock out the inner electrons. If the electrons from the **L** layer fill the vacancies, the energy difference is released as X-ray K_α. If the M-layer electrons occupy the vacancies, K_β will be emitted. $\lambda_{K\alpha} > \lambda_{K\beta}$ The energy difference of K_α is smaller than K_β. According to the following equation, $\nu_{K\alpha} < \nu_{K\beta}$, $\lambda_{K\alpha} > \lambda_{K\beta}$.

$$h\nu = \frac{2\pi^2 m e^4}{h^2}(Z-\sigma)^2\left(\frac{1}{n_2^2}-\frac{1}{n_1^2}\right)$$

(3) K_β will be eliminated (absorbed). The wavelength of the filter (λ_K) should satisfy $\lambda_{K\alpha} > \lambda_K > \lambda_{K\beta}$. If the copper is selected as an anode, the nickel can be used as a filter.

2. (1)



(2)

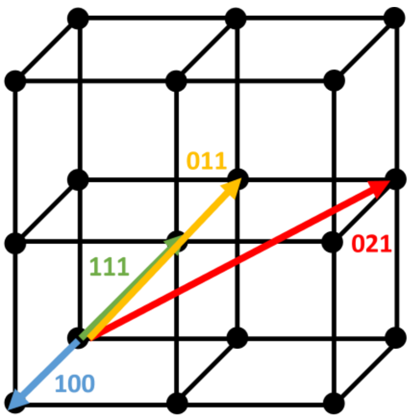
$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$d_{(100)}$ = 0.1 nm, $d_{(011)}$ = 0.071 nm, $d_{(111)}$ = 0.058 nm, $d_{(021)}$ = 0.045 nm

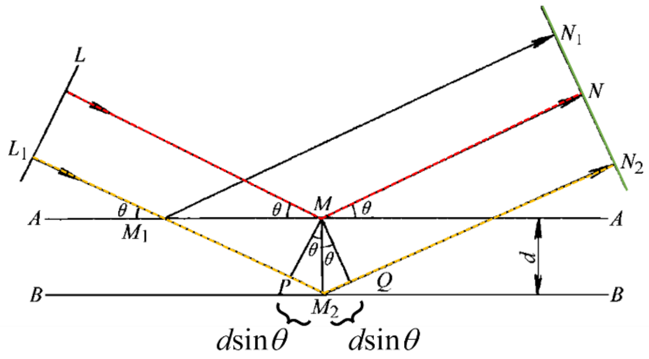
(3)

$$g_{hkl} \perp (hkl), \quad g_{hkl} = \frac{1}{d_{hkl}}$$

g_{100} = 10 nm^{-1}
g_{011} = 14.08 nm^{-1}
g_{111} = 17.24 nm^{-1}
g_{021} = 22.22 nm^{-1}



3. (1)



Displacement difference is $\delta = 2d\sin\theta$

Condition of scattered waves interfere constructively should be: $\delta = n\lambda$

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

(2) $\boldsymbol{\theta}$ is the angle between the incident ray (or reflected ray) and the crystal plane.

d is the interplanar distance.

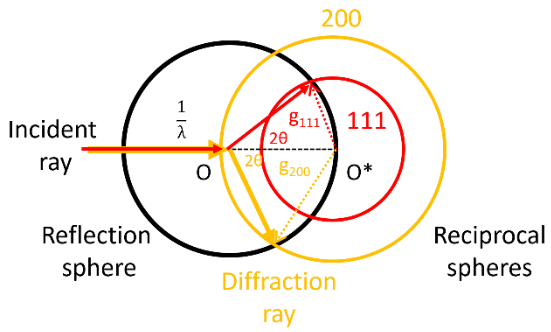
n is called diffraction order.

λ is the wavelength of the X-ray.

(3)

- The d value of the crystal is known. By measuring ***θ***, find the ***λ*** of the characteristic X-ray and use λ to determine the element that produces the characteristic X-ray. This is mainly used in X-ray fluorescence spectrometers and electron probes.
- The wavelength ***λ*** of the incident X-ray is known, and the interplanar spacing can be found by measuring ***θ***. And determine the crystal structure or conduct phase analysis through the crystal plane spacing.

4.



5. (1) $|F_{HKL}|^2$ is called structural factor. It is used to characterize the influence of the atoms' type, number, and position in the unit cell on the (***HKL***) crystal plane diffraction intensity.

(2) There is no system extinction for a simple cubic lattice.

For face-center cubic lattice (FCC), when ***H***, ***K***, and ***L*** are odd and even mixed, $|F_{HKL}|^2 = 0$, and diffraction intensity is zero (system extinction). (100), (110), (210), (300)

For body-centered cubic lattice (BCC), diffraction intensity is zero when ***H*** + ***K*** + ***L***= odd numbers, $|F_{HKL}|^2 = 0$. (100), (111), (210), (300), (311)

(3) $$I = I_0 \frac{\lambda^3}{32\pi R}\left(\frac{e^2}{mc^2}\right)^2 \frac{V}{V_c^2} P|F|^2 \phi(\theta) A(\theta) e^{-2M}$$

I_0 is the intensity of the incident X-ray.
λ is the wavelength of the incident X-ray.
V is the volume of the irradiated crystal.
V_c is the unit cell volume.
P is the multiplicity factor, representing the influence factor of the number of crystal planes on the diffraction intensity.
φ(θ) is the angle factor, which reflects the effect of the size of the grains involved in diffraction in the sample, the number of grains, and the position of the diffraction lines on the diffraction intensity.
A(θ) is the absorption factor. The absorption factor of the cylindrical sample is related to the Bragg angle, the line absorption coefficient ***μ_l*** of the sample and the radius of the sample cylinder; the absorption factor of the flat sample is related to ***μ***, $A(\theta) \propto \frac{1}{2\mu}$ which has nothing to do with ***θ***.

e^{-2M} represents the temperature factor.

6. (1) The accuracy of the lattice parameter a mainly depends on the accuracy of **sinθ**.

(2) Graphical Extrapolation and Least squares method.

7. A piece of cold-rolled steel plate may have three types of internal stress. The first type of internal stress is the stress that exists and remains balanced within a large range of the object or many grains—called macro stress. It can **shift the diffraction lines**.
The second type of stress is the internal stress that exists and remains balanced within one or a few grains. It generally **broadens the diffraction peaks**.
The third type of stress is internal stress, which maintains equilibrium in several atomic ranges. It can **weaken the diffraction rays**.