Homework 1 solution

1. The principle of selecting X-ray tubes in experiments is that to avoid or reduce the generation of fluorescence radiation, you should avoid using X-ray tubes with targets 2 to 6 (especially 2) larger than the atomic number ***Z*** of the main element in the sample.
The principle of filter selection is that in X-ray analysis, a filter should be placed between the X-ray tube and the sample to filter out the K_β line. The material of the filter depends on the material of the target. Generally, a material with an atomic number 1 or 2 smaller than the target is used.
To analyze iron-based samples, choose an X-ray tube with a Co or Fe target and select Fe and Mn as filters, respectively.

2. (100), (110), (111), (200), (121),(220), (030), (130)

3. The effect of the equivalent number of crystal planes on the diffraction intensity is called the multiplicity factor ***P***, and the multiplicity factor is related to the symmetry of the crystal and the crystal plane index. The {100} plane family P = 6 for a cubic crystal system. For tetragonal crystal system, P = 4.

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

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.
F is the structure factor, which reflects the influence factors of the position, type, and number of atoms in the crystal structure on the crystal plane.
$\varphi(\theta)$ 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.
$A(\theta)$ 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.

5. d_{HKL} represents the interplanar spacing of the ***HKL*** crystal plane, θ angle represents the glancing angle or Bragg angle, that is, the angle between the incident X-ray or diffraction line and the specimen, and λ represents the wavelength of the incident X-ray.
This formula has two uses:
(1). 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.

(2). 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.

6. The basic steps for qualitative analysis of single-phase substances are:
(1) Calculate or find each peak's d value and I value on the diffraction pattern.
(2) Use the corresponding d value search index of the three strongest lines with the largest I value to find the name and card number of the phase that basically matches.
(3) Compare the measured d and I values with the data on the card individually. If they are basically consistent, the object can be determined to be in phase.

Issues that should be paid attention to during analysis:
(1) The d data is more important than the I/I_0 data.
(2) Data for low-angle lines is more important than for high-angle lines.
(3) Strong lines are more important than weak lines, and special attention should be paid to strong lines with large d values.
(4) Other analysis and identification methods should be used as much as possible to determine the sample's phase and limit it to a certain range.

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**.