

Appendix 1. The intensity of a single-phase powder specimen in an X-ray diffractometer

The exact expression for the intensity of a single-phase powder specimen in an X-ray diffractometer²³ is

$$I = \left(\frac{I_0 A \lambda^3}{32\pi r} \right) \left[\left(\frac{\mu_0}{4\pi} \right)^2 \frac{e^4}{m^2} \right] \left(\frac{1}{v^2} \right) \left[|F|^2 p \left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right) \right] \left(\frac{e^{-2M}}{2\mu} \right). \quad (1)$$

Here I = integrated intensity per unit length of diffraction line ($\text{joules sec}^{-1}\text{m}^{-1}$), I_0 = intensity of incident beam ($\text{joules sec}^{-1}\text{m}^{-1}$), A = cross-sectional area of incident beam (m^2), λ = wavelength of incident beam (m), r = radius of diffractometer circle (m), $\mu_0 = 4\pi \times 10^{-7} \text{ m kg C}^{-2}$, e = charge on electron (C), m = mass of electron (kg), v = volume of unit cell (m^3), F = structure factor, p = multiplicity factor, θ = Bragg angle, e^{-2M} = temperature factor, and μ = linear absorption coefficient (m^{-1}), which enters as the absorption factor $1/2\mu$. If we put

$$K = \left(\frac{I_0 A \lambda^3}{32\pi r} \right) \left[\left(\frac{\mu_0}{4\pi} \right)^2 \frac{e^4}{m^2} \right] \quad (2)$$

and

$$R = \left(\frac{1}{v^2} \right) \left[|F|^2 p \left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right) \right] e^{-2M}, \quad (3)$$

the diffracted intensity is then given by

$$I = \frac{KR}{2\mu} \quad (4)$$

where K is a constant if the XRD test condition is fixed, R_i depends on the kind and crystallographic orientation of the diffracting substance of the i th layer, and μ is the absorption coefficient of the diffraction substance.²³

For the i th element of a multicomponent system composed of many elements Eq. 4 can be written as

$$I_i = \frac{KR_i}{2\mu_m} C_i \quad (5)$$

where C_i denotes the volume fraction of the i th element and μ_m the absorption coefficient of the multicomponent system.²³ Since absorption is an atomic process, the multicomponent system can be regarded as slabs of each of pure elements as many as the number of the components, that is, a multilayer system.²⁴ In analogy with the expression of Eq. 5, for the i th layer of a multilayer system Eq. 4 can therefore be expressed as

$$I_i = \frac{KR_i}{2\mu_T} C_i \quad (6)$$

where C_i denotes the volume fraction of the i th layer and μ_T the absorption coefficient of the total multilayer system.

Appendix 2. Calculation of the absorption coefficient of the Fe₃O₄ / Fe / Si (100) sample

For a multilayer system the absorption coefficient of the system can be expressed as

$$\mu_T = \sum_i \left[\left(\frac{\mu}{\rho} \right)_i W_i \rho_T \right] \quad (1)$$

where $\left(\frac{\mu}{\rho} \right)_i$ and W_i denote the mass absorption coefficient and weight fraction of the i th layer material, respectively and ρ_T the density of the total system.²⁴ We can write Eq. 2 for a multilayer system consisting of Fe₃O₄ and Fe thin films and an Si substrate:

$$\mu_T = \sum_i \left[\left(\frac{\mu}{\rho} \right)_{Fe_3O_4} W_{Fe_3O_4} + \left(\frac{\mu}{\rho} \right)_{Fe} W_{Fe} + \left(\frac{\mu}{\rho} \right)_{Si} W_{Si} \right] \rho_T \cdot (2)$$

In this system $W_{Fe_3O_4} \approx W_{Fe} \approx 0$ and $W_{Si} \approx 1$ because the Fe_3O_4 and Fe layers are much thinner than the Si substrate, and there is little difference in the $\frac{\mu}{\rho}$ value between them. The absorption coefficient of the sample μ_T can therefore be approximated as

$$\mu_T \approx \left(\frac{\mu}{\rho}\right)_{Si} \rho_{Si} = \mu_{Si} . \quad (3)$$