

2. DIFFRACTION GEOMETRY AND ITS PRACTICAL REALIZATION

 Table 2.6.1.1. Formulae for the various parameters for h (left) and m (right) scales

$R = K\sqrt{\tan \alpha}$ $\tan \alpha = \frac{\Delta \log I(h)}{\Delta h^2}$ $K = \sqrt{\frac{3}{\log e}} = 2.628$	$R = K \frac{\lambda a}{2\pi} \sqrt{\tan \alpha}$ $\tan \alpha = \frac{\Delta \log I(m)}{\Delta m^2}$
$R_c = K_c \sqrt{\tan \alpha}$ $\tan \alpha = \frac{\Delta \log [I(h)h]}{\Delta h^2}$ $K_c = \sqrt{\frac{2}{\log e}} = 2.146$	$R_c = K_c \frac{\lambda a}{2\pi} \sqrt{\tan \alpha}$ $\tan \alpha = \frac{\Delta \log [I(m)m]}{\Delta m^2}$
$R_t = K_t \sqrt{\tan \alpha}$ $\tan \alpha = \frac{\Delta \log [I(h)h^2]}{\Delta h^2}$ $K_t = \sqrt{\frac{1}{\log e}} = 1.517$	$R_t = K_t \frac{\lambda a}{2\pi} \sqrt{\tan \alpha}$ $\tan \alpha = \frac{\Delta \log [I(m)m^2]}{\Delta m^2}$
$V = 2\pi^2 \frac{I(0)}{Q}$ $Q = \int I(h)h^2 dh$	$V = \frac{\lambda^3 a^3}{4\pi} \frac{I(0)}{Q_m}$ $Q_m = \int I(m)m^2 dm$
$A = 2\pi \frac{[I(h)h]_0}{Q}$	$A = \frac{\lambda^2 a^2}{2\pi} \frac{[I(m)m]_0}{Q_m}$
$T = \pi \frac{[I(h)h^2]_0}{Q}$	$T = \frac{\lambda a}{2} \frac{[I(m)m^2]_0}{Q_m}$
$M = \frac{I(0)}{P} K \frac{a^2}{cd(\Delta z)^2}$	$K = \frac{1}{I_e N_L} = 21.0$
$M_c = \frac{[I(h)h]_0}{P} \frac{K}{\pi} \frac{a^2}{cd(\Delta z)^2}$	$M_c = \frac{[I(m)m]_0}{P} \frac{2K}{\lambda} \frac{a}{cd(\Delta z)^2}$
$M_t = \frac{[I(h)h^2]_0}{P} \frac{K}{2\pi} \frac{a^2}{cd(\Delta z)^2}$	$M_t = \frac{[I(m)m^2]_0}{P} \frac{2\pi K}{\lambda^2} \frac{1}{cd(\Delta z)^2}$
$\overline{(\Delta \rho)^2} = \frac{Q}{P} \frac{a^2}{2\pi^2 d} K$ $K = 10^{24}/I_e$ $(10^{24} = [\text{cm}/\text{\AA}]^3)$	$\overline{(\Delta \rho)^2} = \frac{Q_m}{P} \frac{4\pi}{\lambda^3 ad} K$
$O_s = \pi \frac{K}{Q}$ $K = \lim_{h \rightarrow \infty} I(h)h^4$	$O_s = \frac{2\pi^2}{\lambda a} \frac{K_m}{Q_m}$ $K = \lim_{m \rightarrow \infty} I(m)m^4$

$$R_g^2 = \frac{\int_0^\infty p(r)r^2 dr}{2 \int_0^\infty p(r) dr} \quad (2.6.1.17)$$

or from the innermost part of the scattering curve [Guinier approximation (Guinier, 1939)]:

$$I(h) = I(0) \exp(-h^2 R_g^2/3). \quad (2.6.1.18)$$

A plot of $\log[I(h)]$ vs h^2 (Guinier plot) shows at its innermost part a linear descent with a slope $\tan \alpha$, where

$$R_g = K\sqrt{\tan \alpha}$$

(see Table 2.6.1.1).

The radius of gyration is related to the geometrical parameters of simple homogeneous triaxial bodies as follows (Mittelbach, 1964):

sphere (radius R)	$R_g^2 = (3/5)R^2$
hollow sphere (radii R_1 and R_2)	$R_g^2 = (3/5) \frac{R_2^5 - R_1^5}{R_2^3 - R_1^3}$
ellipsoid (semi-axes a, b, c)	$R_g^2 = (1/5)(a^2 + b^2 + c^2)$
parallelepiped (edge lengths A, B, C)	$R_g^2 = (1/12)(A^2 + B^2 + C^2)$
elliptic cylinder (semi-axes a, b ; height h)	$R_g^2 = \frac{a^2 + b^2}{4} + \frac{h^2}{12} = R_c^2 + \frac{h^2}{12}$
hollow cylinder (height h and radii r_1, r_2)	$R_g^2 = \frac{r_1^2 + r_2^2}{2} + \frac{h^2}{12}$

Radius of gyration of the cross section. In the special case of rod-like particles, the two-dimensional analogue of R_g is called radius of gyration of the cross section R_c . It can be obtained from

$$R_c^2 = \frac{\int_0^\infty p_c(r)r^2 dr}{2 \int_0^\infty p_c(r) dr}, \quad (2.6.1.19)$$

where $p_c(r)$ is the PDDF of the cross section or it can be calculated from the innermost part of the scattering intensity of the cross section $I_c(h)$:

$$I_c(h) = I_c(0) \exp(-h^2 R_c^2/2), \quad (2.6.1.20)$$

with $I_c(h) = I(h)h$ (see Table 2.6.1.1).

Radius of gyration of the thickness. A similar definition exists for lamellar particles. The one-dimensional radius of gyration of the thickness R_t can be calculated from

$$R_t^2 = \frac{\int_0^\infty p_t(r)r^2 dr}{2 \int_0^\infty p_t(r) dr}, \quad (2.6.1.21)$$

or from the innermost part of the scattered intensity of thickness $I_t(h)$:

$$I_t(h) = I_t(0) \exp(-h^2 R_t^2), \quad (2.6.1.22)$$

with $I_t(h) = I(h)h^2$ (see Table 2.6.1.1 and §2.6.1.3.2.1).

Volume. The volume of a homogeneous particle is given by

$$V = 2\pi^2 \frac{I(0)}{Q}. \quad (2.6.1.23)$$

This equation follows from equations (2.6.1.12)–(2.6.1.14). Such volume determinations are subject to errors as they rely on the validity of an extrapolation to zero angle [to obtain $I(0)$] and to larger angles (h^{-4} extrapolation for Q). Scattering functions cannot be measured from h equal to zero to h equal to infinity.