POWER-LAW EXPONENT OF FINITE SLIT-HEIGHT/SLIT-WIDTH SMEARED SMALL-ANGLE SCATTERING CURVES

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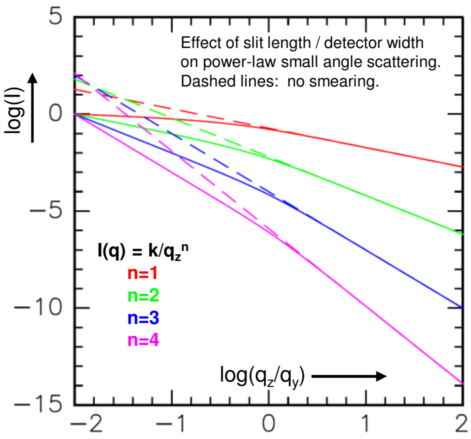
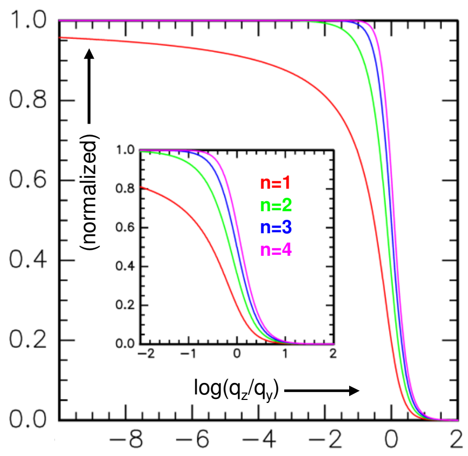
Abstract

Detailed analytical formulas for small-angle scattering curves $I(q_z)$ following a power-law behavior ~ k/q_z^n (with n being the 'Porod exponent' or more generally the power-law exponent) and convoluted by a finite horizontal slit-height and/or detector width (in q_y-direction) have been derived, assuming symmetrically rectangular convolution profiles. It has been shown that the power-law exponent n for q_z-values smaller than the total slit height or detector width quickly decreases and approaches n-1, the limiting value for infinitely long slit profiles [1, 2]. This has consequences for the data evaluation of scattering curves at small angles which were measured by a point-focused beam and a one-dimensional detector with a finite slit-width. The differences between both scattering curves at small angles will be shown and analyzed for a sample, exhibiting a power-law scattering behavior at small q_z-values, which was measured with the same set-up (sample-detector distance ~ 300 mm) with a linear 1D-detector with an 8 mm horizontal opening and with a 2D-detector with 0.17 mm pixel-size, respectively.

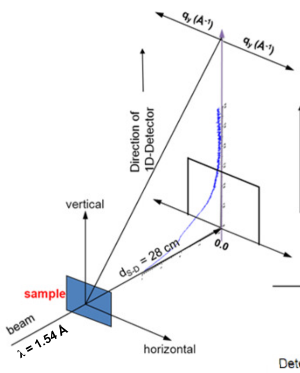
References:
(1) Soler, J. and Baldrian, J. J.Appl.Cryst., 5, 1972, 428-429.
(2) Ciccariello, S. and Sobry, R. J.Appl.Cryst., 32, 1999, 579-589.

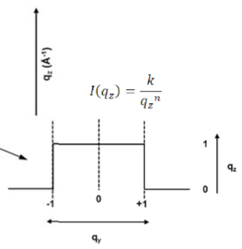




Normalized power-law scattering exponent (slope log(I) vs log(q)) as a function of $\log(q_z/q_y)$ for n = 1 to 4.

Spatial geometry and orientation of X-ray beam, sample and detector





Detector width / Slit height ($-1 < q_y < 1$)

Smearing integrals (power-law scattering curves convoluted by a rectangular horizontal intensity profile):

$$\tilde{I} = 2 \cdot \int_{q_y=0}^{q_y=1} P(q_y) \frac{k}{\left(\sqrt{q_z^2+q_y^2}\right)^n} \cdot dq_y \qquad \text{(equ. 1a)}$$

$$\tilde{I} = 2 \cdot \int_{q_y=0}^{q_y=1} P(q_y) \frac{k}{(q_z^2+q_y^2)^{n/2}} \cdot dq_y \qquad \text{(equ. 1b)}$$

$P(q_y) = 1$ .... $|q_y| \leq 1$ and $P(q_y) = 0$ .... $|q_y| > 1$

General (analytical) solution of the integral (equ. 1) for any n ($x = q_y$):

$$k \cdot 2x \left[\frac{x^2}{q_z^2}+1\right]^{n/2} (q_z^2 + x^2)^{-n/2} \cdot \; {}_2F_1\left[\frac{1}{2}, \frac{n}{2}; \frac{3}{2}; -\frac{x^2}{q_z^2}\right] \Bigg|_{x=0}^{x=1}$$

$$\tilde{I} = \frac{2k \cdot \left(\frac{1}{q_z^2}+1\right)^{n/2} \cdot \; {}_2F_1\left(0.5, \frac{n}{2}; 1.5; -\frac{1}{q_z^2}\right)}{(q_z^2+1)^{n/2}} - 0 \qquad \text{(equ. 2a)}$$

$$\tilde{I} = \frac{2k \cdot \; {}_2F_1\left(0.5, \frac{n}{2}; 1.5; -\frac{1}{q_z^2}\right)}{q_z^n} - 0 \qquad \text{(equ. 2b)}$$

${}_2F_1(a,b;\ c;\ x)$ .... hypergeometric function

$${}_2F_1(a,b;\ c;\ x) = \sum_{i=0}^{\infty} \frac{f_i \cdot x^i}{i!} \quad .....(|x| < 1)$$

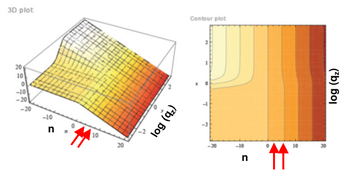
$$f_{i\,(i>0)} = f_{(i-1)} \cdot \left[\frac{((i-1)+a)\cdot((i-1)+b)}{((i-1)+c)}\right] \quad \text{with} \quad f_0 = 1$$

General (analytical) solution of the 1st derivation of the log-log function (equ. 2) for any n ($q_z = 10^x$):

$$\frac{\partial}{\partial x}\left(\log_{10}\left(2\left(\frac{1}{100^x}\right)^{n/2} \; {}_2F_1\left(\frac{1}{2}, \frac{n}{2}; \frac{3}{2}; -\frac{1}{100^x}\right)\right)\right)$$

$$= \left(-\frac{(100^{-x}+1)^{-n/2}}{{}_2F_1\left(\frac{1}{2}, \frac{n}{2}; \frac{3}{2}; -100^{-x}\right)} - n + 1\right) \qquad \text{(equ. 3a)}$$

$$= -\frac{1}{(100^{-x}+1 \quad {}_2F_1\left(1, \frac{3-n}{2}; \frac{3}{2}; -100^{-x}\right)} - n + 1 \qquad \text{(equ. 3b)}$$



3D- and Contour-plots of the slit-smeared power-law exponent for scattering curves $I(q) \sim 1/q_z^n$ as a function of q_z (q_y is set to 1). The SAXS-relevant ranges for n ($1 \leq n \leq 4$) are indicated by red arrows.

General (analytical) solution of the 1st derivation of the log-log function (equ. 2) for any integer n ($q_z = 10^x$):

	$\tilde{I}$		$\frac{d\log(\tilde{I})}{dx}$
all n	$\frac{2k \cdot \; {}_2F_1\cdot\left(\frac{1}{2}, \frac{n}{2}; \frac{3}{2}; -\frac{1}{x^2}\right)}{x^n}$	$\rightarrow$	$-\frac{1}{\left(\frac{1}{(10^x)^2}+1\right)^{n/2} \; {}_2F_1\left(\frac{1}{2}, \frac{n}{2}; \frac{3}{2}; -\frac{1}{(10^x)^2}\right)} - n + 1$
n = 5	$\frac{2k \cdot (3x^2+2)}{3x^4 \cdot \sqrt{(x^2+1)^3}}$	$\rightarrow$	$-\frac{3 \cdot (10^x)^4}{(3 \cdot (10^x)^4 + 5 \cdot (10^x)^2 + 2)} - 4$
n = 4	$\frac{2k \cdot \left(\frac{x}{x^2+1} + \tan^{-1}\left(\frac{1}{x}\right)\right)}{2x^3}$	$\rightarrow$	$-\frac{2 \cdot (10^x)^3}{10^x + (10^x)^3 + ((10^x)^2+1)^2 \tan^{-1}\left(\frac{1}{10^x}\right)} - 3$
n = 3	$\frac{2k}{x^2 \cdot \sqrt{x^2+1}}$	$\rightarrow$	$-\frac{(10^x)^2}{(10^x)^2+1} - 2$
n = 2	$\frac{2k \cdot \tan^{-1}\left(\frac{1}{x}\right)}{x}$	$\rightarrow$	$-\frac{10^x}{((10^x)^2+1)\tan^{-1}\left(\frac{1}{10^x}\right)} - 1$
n = 1	$2k \cdot \ln\left(\frac{1+\sqrt{1+x^2}}{x}\right)$	$\rightarrow$	$-\frac{1}{\sqrt{1+(10^x)^2} \cdot \ln\left(\frac{1}{10^x}\cdot\left(1+\sqrt{1+(10^x)^2}\right)\right)} - 0$

'Porod constant k' for slit-smeared scattering curves ($\tilde{n} = n - 1$ if slit q_y is inifinitely long)

$I(q) = k/q^n$ $\tilde{I}(q) = \tilde{k}/q^{\tilde{n}}$	limiting value for k (infinitely long slit)	$k = a \cdot \tilde{k}$
n = 5	$4/3$	$k = 3/4 \cdot \tilde{k}$
n = 4	$\pi/2$	$k = 2/\pi \cdot \tilde{k}$
n = 3	2	$k = 1/2 \cdot \tilde{k}$
n = 2	π	$k = 1/\pi \cdot \tilde{k}$
n = 1	∞	-

S_i (inner surface, area/volume) for n = 4 and $\tilde{n}$ = 3, respectively:

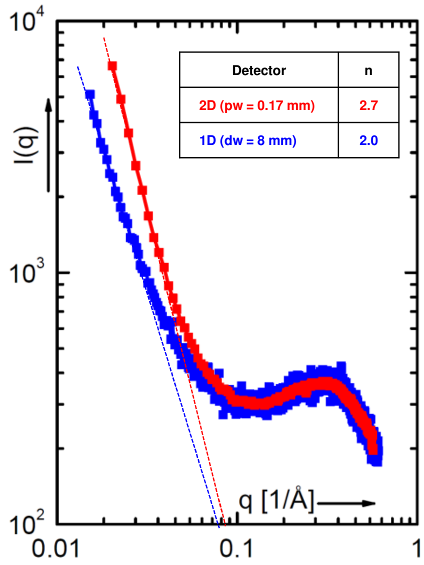
$$S_i = \pi \cdot k/Q \qquad S_i = 4 \cdot \tilde{k}/\tilde{Q}$$
$$S_i = 2 \cdot \tilde{k}/Q \qquad S_i = 2\pi \cdot k/\tilde{Q}$$

where: $Q = \tilde{Q}/2$ and $k = 2 \cdot \tilde{k}/\pi$

with the 'invariant' Q:

$$Q = \int_0^{\infty} I(q) \cdot q^2 \cdot dq$$

$$\tilde{Q} = \int_0^{\infty} \tilde{I}(q) \cdot q \cdot dq$$



SAXS-curves of a coal sample measured with a point-source and a 1D-detector (horizontal width: 8 mm) and a 2D-detector (pixel-size: 0.17 mm).

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