Quantitative small angle scattering on mesoporous silica powders: from morphological features to specific surface estimation

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1. Effect of the pore number on the SAXS profile of hexagonal mesoporous silica

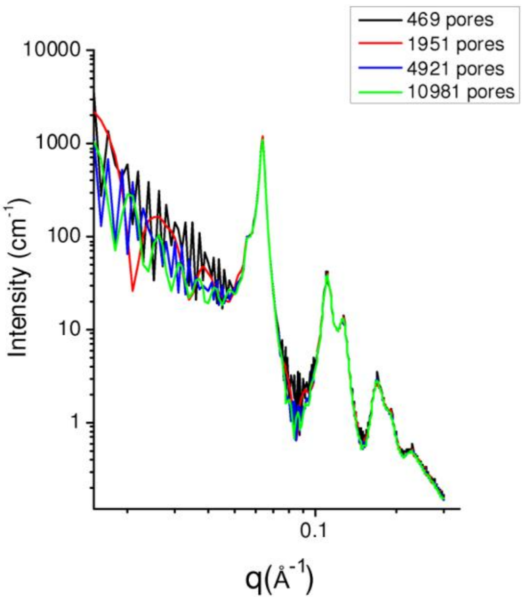

Figure S1: Calculated SAXS profile of porous silica containing hexagonal lattices of 469, 1951, 4921, and 10981 pores (corresponding respectively to 12, 25, 40, and 60 concentric shells of pores), assuming a pore radius of 45 Å, a lattice parameter of 113 Å, and a degree of paracrystallinity of 20%. The data were not convoluted with an experimental resolution.

2. Detail of the formalism for SAXS intensity calculations

We start from the following equations presented in the article body, the different quantities are defined in the text.
The general intensity is given by equation:

$$I(q) = \frac{\iint_{S_q} \left| A(\vec{q}) A^*(\vec{q}) \right| dS_q}{4\pi q^2} \qquad (16)$$

The scattering amplitude of a porous grain can be written as:

$$A(\vec{q}) = A_g(\vec{q}) - \sum_{Np} A_p(\vec{q}) \,, \qquad (13)$$

with

$$A_g(\vec{q}) = \frac{2\pi\rho_b L}{q\sin u}\frac{\sin\left(q\cos u\frac{L}{2}\right)}{q\cos u\frac{L}{2}}R_g J_1\left(R_g q\sin u\right), \tag{14}$$

and

$$A_g(\vec{q}) = \frac{2\pi\rho_b L}{q\sin u}\frac{\sin\left(q\cos u\frac{L}{2}\right)}{q\cos u\frac{L}{2}}R_g J_1\left(R_g q\sin u\right) \tag{15}$$

$A_g(\vec{q})$ is the scattering amplitude of a cylindrical grain of dense non-porous material, and $A_p(\vec{q})$ is the scattering amplitude of one pore in the grain.

Considering equations (13), (14), and (15), one can write:

$$A(\vec{q})\cdot A^*(\vec{q}) = T\cdot M \tag{1*}$$

with $A^*(\vec{q})$ the complex conjugate of $A(\vec{q})$, and T and M expressed as:

$$T = \frac{\rho_b{}^2 4\pi^2 L^2}{q^2\sin^2 u}\frac{\sin^2\left(q\frac{L}{2}\cos u\right)}{\left(q\frac{L}{2}\cos u\right)^2} \tag{2*}$$

$$M = \left[R_g J_1(R_g q\sin u) - \sum_i e^{-iqR_i \sin u\cos(\psi-\varphi_i)}R_p J_1(qR_p\sin u)\right]\left[R_g J_1(R_g q\sin u) - \sum_j e^{-iqR_j \sin u\cos(\psi-\varphi_j)}R_p J_1(qR_p\sin u)\right] \tag{3*}$$

with φ_i and φ_j being angles between the x-axis and the vectors R_i and R_j pointing towards the centre of tubes i and j, respectively.

When the length L of tubes becomes very large, the following property of the Dirac function can be used:

$$\lim_{\varepsilon\to 0^+}\left(\frac{\varepsilon}{\pi}\frac{\sin^2\left(\frac{x}{\varepsilon}\right)}{x^2}\right) = \delta(x) \tag{4*}$$

The T term thus writes:

$$T = \frac{8\pi^3 L\rho_b{}^2}{q^3\sin^2 u}\delta(\cos u) \tag{5*}$$

Equation (5*) imposes that T is non-zero only when u = π/2. We can therefore write the expression of the intensity per length unit I(q)/L by combining equations (16), (3*) and (5*):

$$\frac{I(q)}{L}=\frac{2\pi^2\rho_b^2}{q^3}\left[2\pi R_g^2 J_1^2(qR_g)-2R_g J_1(qR_g)R_p J_1(qR_p)\sum_i\int_{\psi=0}^{2\pi}\cos(qR_i\cos(\psi-\varphi_i)d\psi+R_p^2 J_1^2(qR_p)\sum_{i,j}\int_{\psi=0}^{2\pi}e^{iqR_{ij}\cos(\psi-\varphi_{ij})}d\psi\right.$$

(6*)

and introducing J_0 Bessel functions in place of the summations over ψ, one obtains equation (17) presented in the text.

From equation (6*), it is directly visible that the double sum over pores is made over an exponential term of the form $e^{i\vec{q}\overrightarrow{R_{ij}}}$. When considering the paracrystal model presented in paragraph 4.2, it is possible to use equation (22) in order to replace the exponential summation by the Z(q) function described in equation (19).