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SAXS100 and SAXS200. A software package for PC

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The intent is to present a new software package for Small-Angle X-ray Scattering (SAXS) which offers a user-friendly approach for data analysis using a low-cost personal computer. The software package is suitable for any collimation conditions including the special cases of a point-like primary beam as well as of an infinitely long primary beam. Other features of the programs include: direct calculation of different kinds of structure functions (e.g. correlation function of electron density $C(r)$, chord distribution function $A(l)$, particle size distribution $N(d)$); calculation of characteristic structure parameters (e.g. electronic radius of gyration, correlation length, correlation area, correlation volume, average electron distance); various plots of tails and analytical evaluations; fitting of the smeared and the desmeared scattering curves according to a damped Newtonian procedure with different analytical expressions.

Introduction

Most experimental systems for measuring Small Angle X-ray Scattering (SAXS) employ slit collimation in order to provide sufficient scattering intensity. As result, a scattering curve, called the smeared curve, is obtained. This collimation distortion is described by

$$\hat{I}(s) = \int W_h(u) \cdot I(s-u) du \quad (1)$$

$$\tilde{I}(s) = \int W_w(u) \cdot \tilde{I}(\sqrt{s^2 + u^2}) du, \quad (2)$$

where $\hat{I}(s)$ is the measured intensity, $\tilde{I}(s)$ is the intensity distorted by slit length and $I(s)$ is the unsmeared intensity; $s = 4\pi/\lambda \cdot \sin(\Theta)$, λ - wavelength and 2Θ is the scattering angle. The function $G(s)$ is the convolution of the width of the detector slit and the primary beam-width intensity profile in the detector plane. The slit-length weighting function $P(t)$ is the convolution of the length of the detector slit and the primary-beam-length intensity profile. For the special cases of as of an infinitely long primary beam and a neglected width smearing the equation (2) can be simplified:

$$\tilde{I}(s) = 2 \int_0^\infty I(\sqrt{s^2 + u^2}) \cdot du \quad (3)$$

All information about the scattering sample obtainable from small-angle scattering data is contained in the discrete measured points of a measured curve, provided that the interval Δs between adjacent measured points fulfils the condition $\Delta s \leq \pi/L$, where L is the largest correlation distance in the sample. The consistent utilization of this principle leads to our software package.

Theory

The correlation function $C(r)$ is obtained from scattered intensity for pinhole collimation

$$I(s) = \frac{1}{2 \cdot \pi^2} \int_0^\infty I(s) \cdot s^2 \frac{\sin(sr)}{sr} \cdot dr \quad (4)$$

For the special cases of an infinitely long primary beam we get with (3) in consideration of Δs smaller than the sampling point distance:

$$C(r) = \sum_{k=1}^{k_{\max}} \Delta s^2 \cdot k \cdot \tilde{I}(k \cdot \Delta s) \cdot Z(k, \Delta s \cdot r) + C_e(r) \quad (5)$$

with

$$Z(k, y) = \frac{2}{\pi} \int_0^{\sqrt{x^2 - y^2}} \frac{\sin(k \cdot \sqrt{y^2 + x^2})}{\sqrt{y^2 + x^2}} \cdot dx \quad (6)$$

Figure 1 shows that $Z(k, y) \approx J_0(k \cdot y)$ for large k . For small k a non neglected error arise by using the Besselfunction. Experimental scattering curves can be measured only in a finite range of the variable s . To reduce the termination effect a scattering curve may be extended by an expression of the form $\tilde{I}(s) = K/s^3$, where K is the tail constant. The correction term of (5) obtained by this extrapolation is

$$C_e(r) = \frac{K}{4 \cdot \pi^2} \int_{s_{\max} + \Delta s/2}^\infty \frac{J_0(sr)}{s^2} \cdot dr \quad (7)$$

The collimation correction is automatically carried out with the calculation of the correlation function by equation (6). A technique has been developed too for correcting small-angle X-ray scattering curves for the distortions produced by any width and length of the collimating slits. The method is based on applying the frequency function, which can be calculated from discrete measured points:

Figure 1: Comparision of the Besselfunction and function equitoiin (6)

$$F(r) = \Delta s \frac{\hat{I}(0)}{2} + \sum_{k=1}^{k_{\max}} \Delta s \cdot \hat{I}(k \cdot \Delta s) \cdot \cos(k \cdot \Delta s \cdot r) + F_e(r) \quad (8)$$

where $F_e(r)$ describes the correction of the termination effect.

$$F_e(r) = K \int_{s_{\max} + \Delta s/2}^{\infty} [\cos(s \cdot r) / s^n] ds \quad (9)$$

When this function is divided by the Fourier transform of the slit-width weighting function, the slit-width corrected frequency function is obtained. The slit-length corrections makes use of slit functions calculated by /3,4/. Then the slit-length corrected scattering curve is evaluated from the analytically differentiated slit-width-corrected intensity function by numerical integration:

$$I(k \cdot \Delta s^*) = [\tilde{F}(0) / \pi] \cdot \Delta r + \sum_{j=1}^{j_{\max}} (2 \cdot \Delta r / \pi) \cdot \tilde{F}(j \cdot \Delta r) \cdot Q(k \cdot \Delta s^*, j \cdot \Delta r) \quad (10)$$

with

$$Q(k \cdot \Delta s^*, j \cdot \Delta r) = \cos(j \cdot k \cdot \Delta r \cdot \Delta s^*) + (j \cdot \Delta r / \pi) \cdot \quad (11)$$

$$\cdot \int_0^{t_{\max}} H^*(t) \cdot \sin \left\{ j \cdot \Delta r \left[(k \cdot \Delta s^*)^2 + t^2 \right] \right\}^{1/2} \cdot \left[(k \cdot \Delta s^*)^2 + t^2 \right]^{-1/2} dt$$

The latter intensity, which is partially smoothed, is calculated from the slit-width-corrected frequency function by a series of expression. By use of the same technique, an adequate expression for calculating the collimation-corrected scattering curve for the case of infinitely long slit collimation was derived.

Software description

The software is written in C using the MS-DOS operating system and has been tested on various generations of PC computers (80286, 80386 and 80486) having at least 1 MB memory and a black and white VGA monitor with a resolution of 640x480 pixels. The programs are characterized by an integrated graphical environment including menu control (keyboard, mouse, trackball), which is advantageous also for novice users because no difficult commands have to be memorized. The standard features are pop-up menus for easy control of events (fig. 2), short on-line hints for obtaining help, display of scattering and structure functions on the screen in a graphical mode (fig. 3) with the possibility of further data evaluations (extrapolation, damping, data reduction, fitting, graphical comparison of results, parameters calculation).

Fig. 2: Pop-up-menu for the graphical representation of the results

Fig. 3: Calculated correlation function normalized to one and a corresponding alert-box for controlling events by the user at this stage of data treatment

Interested persons in application of the software package can get further information from the authors.
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