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A new package: MySAS for small angle scattering data analysis

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Abstract In this paper, A MySAS package, which is verified on Windows XP, can easily convert two-dimensional data in small angle neutron and X-ray scattering analysis, operate individually and execute one particular operation as numerical data reduction or analysis, and graphical visualization. This MySAS package can implement the input and output routines via scanning certain properties, thus recalling completely sets of repetition input and selecting the input files. On starting from the two-dimensional files, the MySAS package can correct the anisotropic or isotropic data for physical interpretation and select the relevant pixels. Over 50 model functions are fitted by the POWELL code using χ^2 as the figure of merit function.

Key words Data analysis, Small angle scattering, SANS, SAXS, MySAS package.

1 Introduction

The two-dimensional (2D) and position-sensitive detector (PSD) has been widely used for small angle neutron and X-ray scattering (SANS and SAXS, usually SAS)[1] to improve radiation detection of samples. The corresponding 2D data is required to convert into one-dimensional curve by programs, such as SANS_analysis[2], ATSAS[3], FISH[4], canSAS[5], BerSANS[6], and GRASP[7], but the 2D pattern is usually complex due to the anisotropic diffuse scattering and Bragg peak at large angles. In order to reduce the 2D scatters and correct the anisotropic or isotropic data completely, a Pxy package[8] can solve partly the anisotropic of SAS 2D pattern. In this paper, a MySAS package for treating SAS 2D feature is developed. Each step of the filter setting, model fitting, and result reporting can be fulfilled by mouse click or line command.

2 Primary data processing

The position-sensitive detector with wave vector of $2\pi/\lambda$ ($\boldsymbol{k}_i$) is flatly perpendicular to the beam, where λ is wavelength. Each detector pixel determines a direction of elastic scattering beam with wave vector ($\boldsymbol{k}_f$) and scattering angle (2θ). The scattering vector ($\boldsymbol{q}$) is defined as $\boldsymbol{q} = \boldsymbol{k}_f - \boldsymbol{k}_i$, and $|\boldsymbol{q}| = (4\pi/\lambda)\sin\theta$.

The 2D data analysis includes loading data files, displaying data, picking pixels, converting the pixels to curve, and fitting the curve and saving result, as shown in Fig.1.

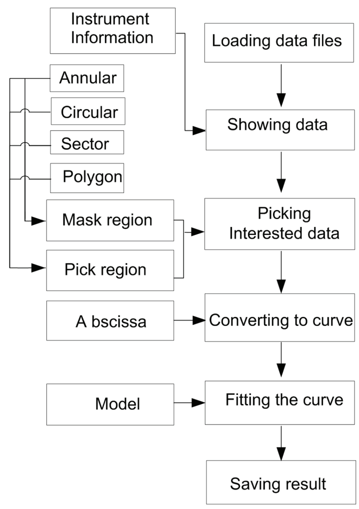

Fig.1 Flow chart of the MySAS package.

Fig.2 shows the five parts of functions in the user interface of MySAS package, i.e. Part(a), the Graph 2D, which serves for displaying data and

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interested pixels; Part(b), the curve fitted with required pixels; Part(c), parameter setting of the SAS model; Part (d) the data processing; and Part(e), the command in three table pages, with the SAS in side expressing relevant information with kernel and macro-control. The command in Part(f) is a line editor. The five sections can be easily snapped individually by some toolbars, and all the controls are implemented by clicking mouse and keyboard commands.

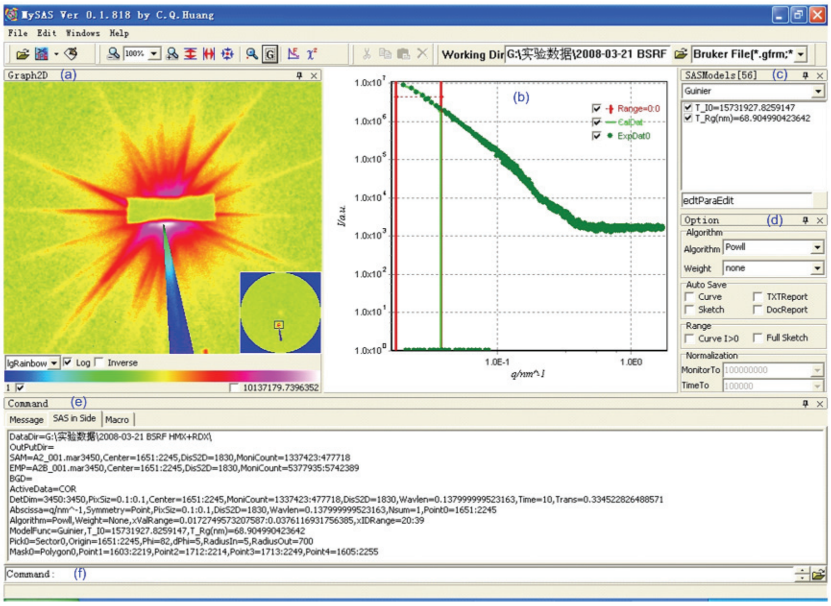

Fig.2 The graphical user interface of MySAS package. (a) 2D data displaying, (b) fitted curve, (c)model settings, (d)data processing, (e) three table pages expressing relevant information in kernel and macro-control, (f) a line-command editor.

2.1 Loading data files

Fig.3 shows that the MySAS package can be used for reading data files in many laboratories and some Bruker machines with TIFF image format and uncompressed binary file. The input-data file includes empty container (EMP), background (BGD), and sample (SAM). The instrument parameters, such as wavelength and monitor counts, can be specified and modified by the control command.

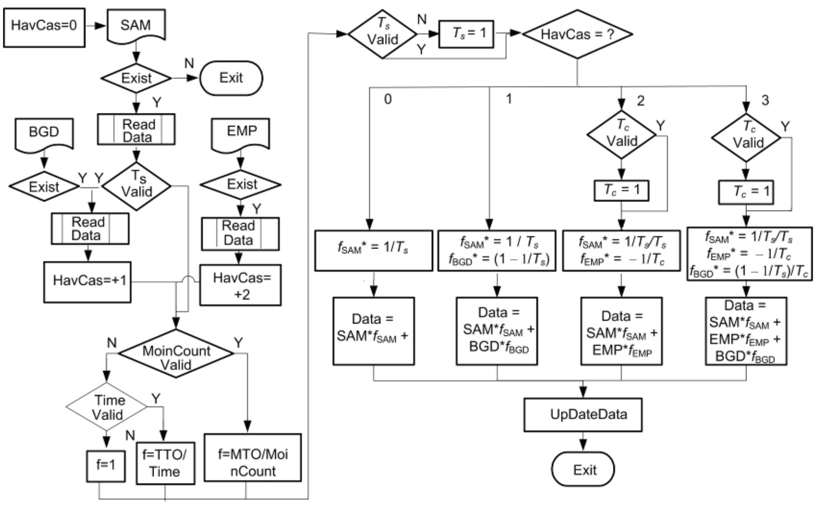

Fig.3 **A** scheme of data correction, the transmission of sample container (T_s) and empty container (T_c), the normalized values of time (TTO) and monitor (MTO).

2.2 Displaying the data

All active data are displayed and manipulated by an active-data command, such as SAM, EMP, BGD and corrected data (COR). Setting the COR shown in Fig.3, the 2D data can be corrected by the MySAS package. Otherwise, the corresponding data is directly loaded from the specified file.

To eliminate background contribution and obtain the real intensity of scatterings from the sample, the sample transmission with the container (T_s) and empty container (T_c) is required. According to the scheme of experiment in Fig.4, the real intensity ($I_{SAM:r}$) scattered from the sample depends on the T_s and T_c, and is given by Eq.(1),

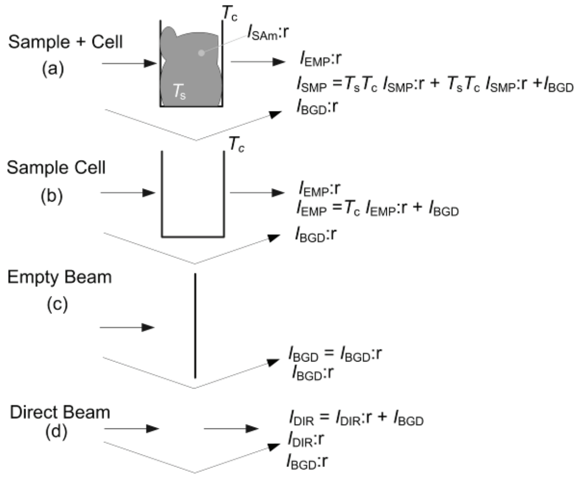

Fig.4 Scheme of the SAS measurement.

$$I_{\text{SAM:r}} = \frac{1}{T_s}\left(I_{\text{SAM}} - I_{\text{BGD}}\right) - \frac{1}{T_c}\left(I_{\text{EMP}} - I_{\text{BGD}}\right) \quad (1)$$

where T_c and T_s are calculated by

$$T_c = \frac{I_{\text{EMP:r}}}{I_{\text{DIR:r}}} = \frac{I_{\text{EMP}} - I_{\text{BGD}}}{I_{\text{DIR}} - I_{\text{BGD}}} \quad (2)$$

$$T_s = \frac{I_{\text{SAM:r}} + I_{\text{EMP:r}}}{I_{\text{DIR:r}}} = \frac{I_{\text{SAM}} - I_{\text{BGD}}}{I_{\text{DIR}} - I_{\text{BGD}}} \quad (3)$$

where, I_{SAM}, I_{EMP}, I_{BGD}, and I_{DIR} refer to the normalized detector counts of sample container, empty container, background, and direct beam, respectively; while $I_{SAM:r}$, $I_{EMP:r}$, $I_{BGD:r}$, and $I_{DIR:r}$ refer to the contribution to detector counts of the sample container, empty container, background and direct beam, respectively. Without the sample container, the beam intensity for empty container is the same as the direct beam, i.e. at I_{EMP}=I_{DIR} and T_c=1, the Eq.(1) is true, too.

Fig.4 shows that the intensity associates with seven color map defined in the program, thus displaying at least 200 levels. The user can associate the color map with I(or lg$I$) in order to enhance details. Both useful and useless pixels are specified in the pick or mask region, and the interested pixels are highlighted in inverse color map.

2.3 Picking the interested data

Indeed, not all pixels are useful. It is very important for the filter to select and design the useful pixels. Fig.5 shows that the four primary regions are defined, and all interested pixels are labeled into summation or subtraction as pick or mask without quantitative restriction regions.

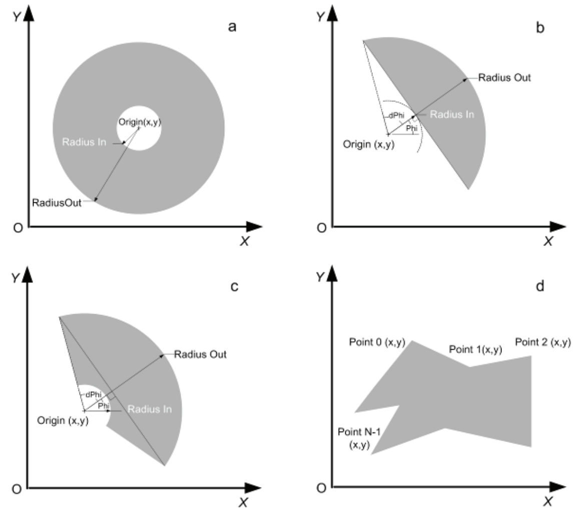

Fig.5 Primary picking region.
(a) annular, (b) chord, (c) sector, (d) polygon.

2.4 Converting the picked pixels to curve

The data of picked pixels are converted into a curve by the scheme of abscissa settings (Fig.6). Parameters of abscissa include its unit (i/pixel, q/nm^{-1}, r/mm or theta/°) and symmetry (point or line), and the interested pixels are categorized in certain abscissa bin. The converted curve and the process information are saved as a file at any time of the whole analyzing.

2.5 Fitting the curve

The MySAS package implements all the SAS models in SANS_Analysis developed by R. K. Steven[2] and other model-independent functions (Guinier, Porod, Zimm, Debye, Fractal[1]). Note that other programs can also be employed to fit the converted curve, such as ORIGIN, EXCEL, and IGOR. In MySAS, the fitting process is the well-known POWELL algorithm[9] with a figure of merit function. The object function is χ^2 with or without weighting of error and value of intensity.

2.6 Saving results

Once the fitting finished, its results can be saved as image or text file with all process information, and brilliantly expressed by other software like Origin. A history file will be created at the exit of MySAS, with which the results achieved can be reproduced.

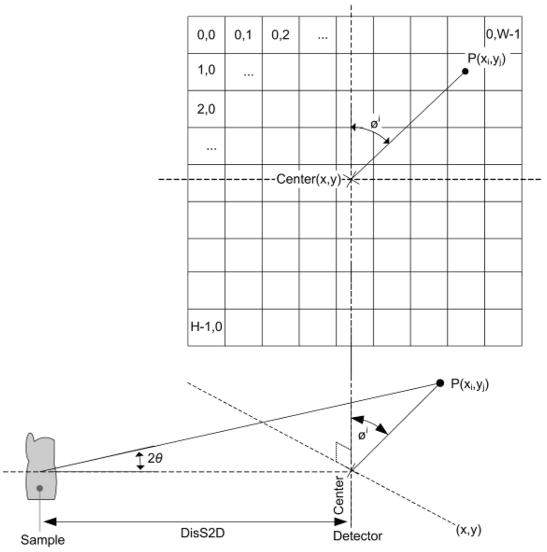

Fig.6 The geometrical relation of sample-detector.

3 Examples

MySAS package was use to analyse two kinds of examples, the isotropic and the anisotropic, to validate its ability.

3.1 The isotropic sample

Fig.7 shows that the scattered SAXS patterns of CL-20 [10] particles, which were produced by different treatments, changing from the isotropic to the anisotropic due to the re-crystallization. The average scattering curves were obtained by an azimuthally annular filter. If the scatters are a polydisperse population of spheres with uniform scattering length density (SLD) at the distribution of Gaussian radii, this can be given by Eq.(4)

$$I(q)=(\frac{4\pi}{3})^2 N_0\Delta\rho^2\int_0^\infty f(R)R^6[\frac{\sin(qR)-qR\cos(qR)}{(qR)^3}]^2\,\mathrm{d}R \quad (4)$$

where, N_0 is the total number of scatters per unit volume, $\Delta\rho$ is the SLD difference, and $f(R)$ is Gaussian distribution,

$$f(R)=\frac{1}{\sigma\sqrt{2\pi}}\exp[-\frac{1}{2\sigma^2}(R-R_{avg})^2] \quad (5)$$

where R_{avg} is the average radius, and $p = \sigma/R_{avg}$ is the polydispersity, and its physical properties are interpreted by the parameters of this model.

Fig.7a–7c shows that the scatters depend on the crystal structure, and the crystal grain is perfected by the treatment. In general, a large uncertainty in high q ranges cannot be fitted well by the SAS analysis. Fig.7d shows the converted data (dot) and the fitted model curve (solid). From the model parameter, it can be concluded that the volume fraction of scatter decreased due to sedimentation and evaporation, and the size and distribution are not nearly changed, this is consistent with the macro properties based on defects theory.

After treating the samples by the SANS_ Analysis, the R_{avg} is 37.25, 37.58, and 37.86 nm, p is 0.21, 0.20, and 0.19, and volume fraction is 1.59, 1.35, and 1.12, respectively.

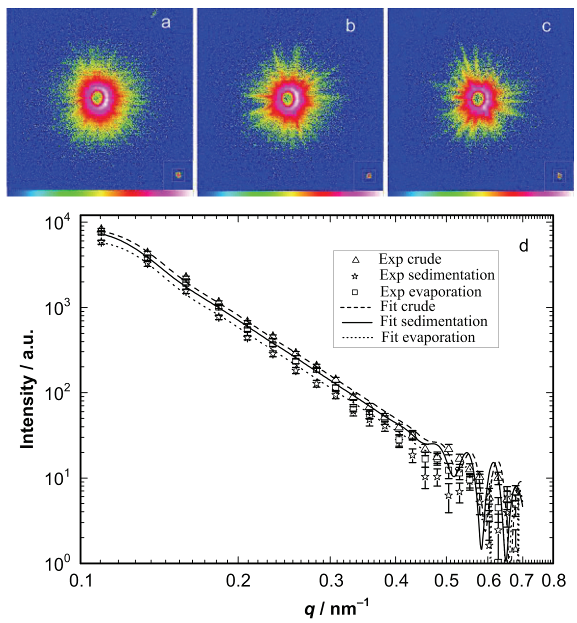

Fig.7 SAXS patterns of CL-20 (2, 4, 6, 8, 10, 12-hexanitro-2, 4, 6, 8, 10, 12-hexaazaisowurtzitane, HNIW) corrected with treatment of (a) the crude,(b) re-crystallized by sedimentation and (c)evaporation. The data converted from an annular region (dot) and fitted model curve (solid) are given in Fig.7(d).

3.2 The anisotropic sample

When the SAS experiment provides an anisotropic scattering pattern, the filtering procedure needs be carefully designed. Fig.8 shows that the SAXS pattern of sensitivity scattering deduced the RDX[11]. In order to evaluate the scatter size, the two groups of sectors are chosen as pick filter. Azimuthally, the six sectors belong to the valleys, and another such six sectors to the ridges. A polygon as mask filter is used to eliminate the beam stop projection on the PSD.

Fig.8(d) shows that the intensity curves of fitted valleys and ridges with poly disperse population of spheres and uniform scattering length density change with scattering vector. On fitting valley and ridge of poly disperse spheres via the distribution of Gaussian radii, their typical scatter R_{avg} are 41.22 and 88.70 nm with 0.77 and 0.31 of poly dispersity, respectively. In contrast, fitted by SANS_Analysis, their average scatter R_{avg} are 39.8 and 88.51 nm, the poly dispersity is 0.72 and 0.31, and volume fraction is 29.83 and 799.28, respectively. This discrepancy may be caused from fitting algorithm, data range, and precision.

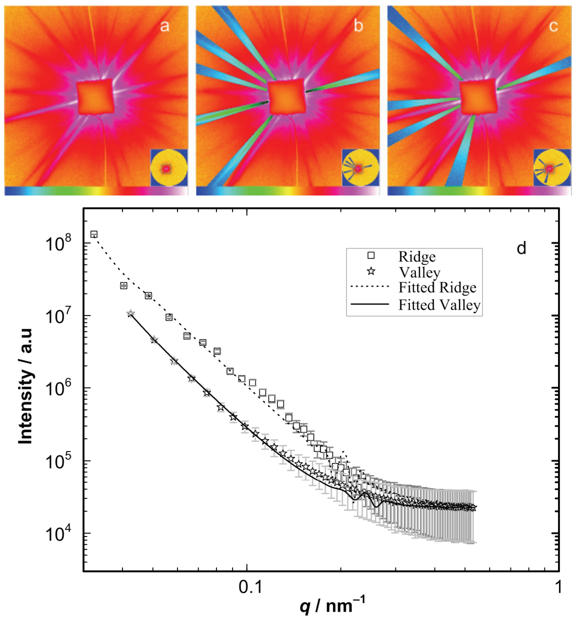

Fig.8 SAXS analysis of a sensitivity deduced RDX. (a) the corrected SAXS pattern, (b) the azimuthally region of the scattering pattern in ridge, (c) valley, (d) the intensity curves of fitted valleys and ridges changing with scattering vector. The background is 22000 and the difference in scattering length density is 2.06×10^{-4} nm^{-2}.

4 Conclusions

The basic concept of MySAS package is explained, including data correction, versatile filter design, model function used in one-dimensional fitting and few usages. The user with macro-mode can analyze all kinds of data quickly and conveniently. The MySAS package illustrated by two examples is applied to analyze the isotropic and the anisotropic. As better SAXS resolution than SANS's the resolution can be neglected for SAXS but cannot for SANS, and the combined analysis of fitting performance with multiple data and resolution will be further studied and improved by the CONDOR[12] optimizer of F.V. Berghen.

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