FitGISAXS manual

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1 Introduction

FitGISAXS is a software package for performing modelling and analysis of GISAXS data within the distorted wave Born approximation (DWBA). The tool suite uses a slab-model approach with the Abeles matrix method to calculate X-ray reflectivity curves, electric field intensity distributions as well as GISAXS intensities from supported or buried scatterers arranged in 2 or 3 dimensions in a stratified medium. Models are included to calculate the scattered intensity for monodisperse, polydisperse, and interacting particles with various size distributions, form factors and structure factors. The source code for the entire package is freely available, allowing anyone to develop additional tools.

FitGISAXS works within the version 6 of IGOR Pro (Wavemetrics, OR), which is an integrated program for visualizing, analyzing, transforming and presenting experimental data. You don't need to purchase IGOR in order to use the functions, a free demo version is available from their website. FitGISAXS will work just as well in the demo version, as the full version.

2 Installing FitGISAXS

1. Install IGOR Pro by downloading from the Wavemetrics website (`www.wavemetrics.com`).
2. Copy the \Procedures_GISAXS directory in your \WaveMetrics\Igor Pro 6 User Files\Igor Procedures directory.
3. Copy the \User_GISAXS directory in your \WaveMetrics\Igor Pro 6 User Files\User Procedures directory.
4. Launch Igor Pro 6 and click on FitGISAXS_5 in the Macros menu. Once the procedures have compiled then a FitGISAXS menu should appear on the top menu as well as 3 'yellow' windows which can be used to fix the input parameters for performing modelling and analysis of GISAXS data (see Fig. 1).

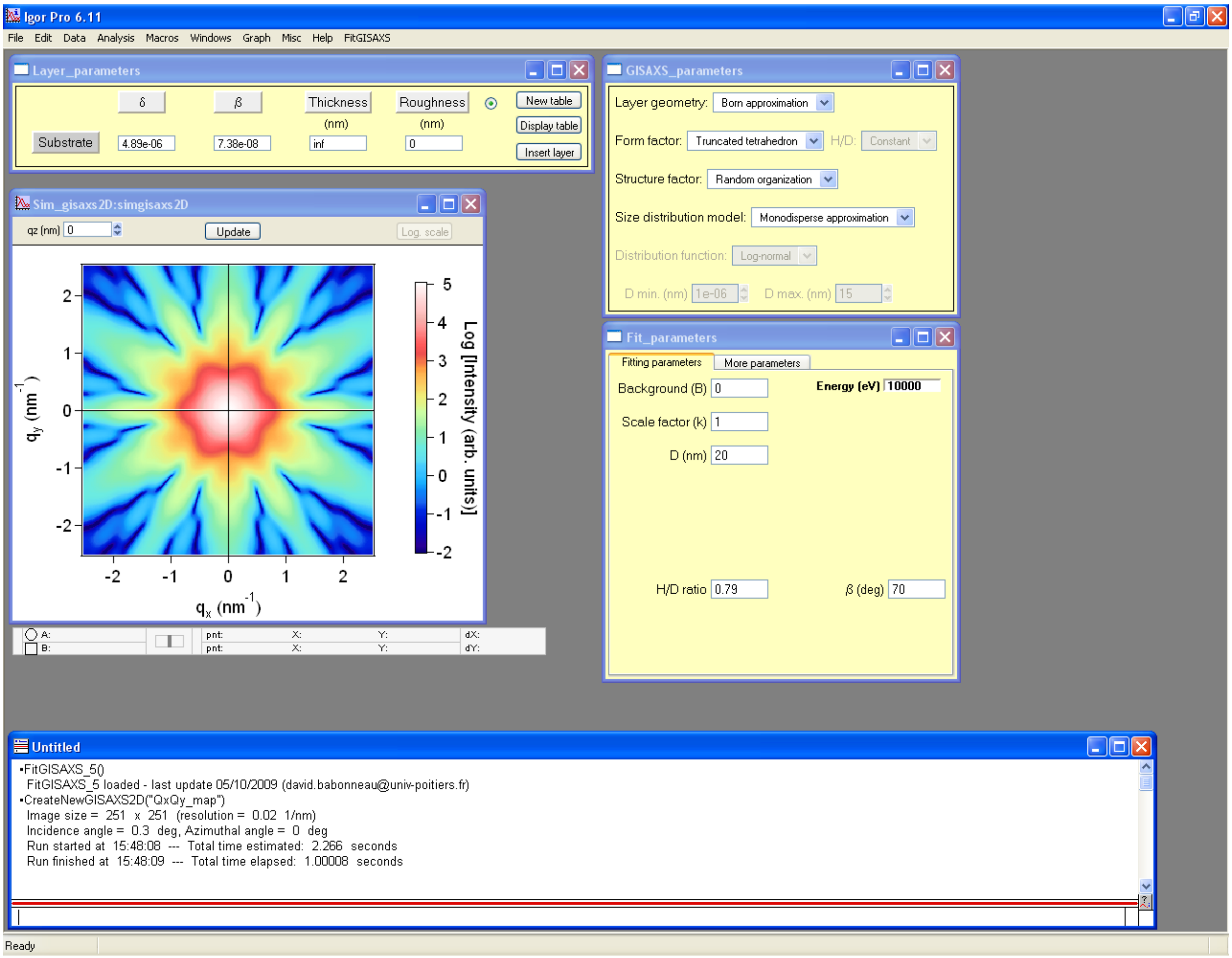

FIGURE 1 – A screen shot of the user interface.

3 Layer_parameters window

The reflectivity, electric field intensity distribution, and GISAXS intensity are calculated using the Abeles matrix method [1]. It is considered that a plane wave $E_0^-(\vec{r},t) = A_0^-(\vec{r})e^{i(\omega t - \vec{k}_0^- \vec{r})}$ impinges on the surface ($z_1 = 0$) of a stratified medium consisting of $N-1$ layers supported by a semi-infinite substrate, as illustrated in Fig. 2. The air and the substrate are labelled as medium 0 and N, respectively, and their refractive indices are $n_0 = 1$ and $n_N = 1 - \delta_N - i\beta_N$. Each layer j ($1 \leq j \leq N-1$) is characterized by its refractive index $n_j = 1 - \delta_j - i\beta_j$ and its thickness t_j. The roughness of the interface z_j between the $j-1$ and j layers is σ_j assuming a Gaussian height probability distribution.

All the δ_j, β_j, t_j, and σ_j parameters can be included in the Layer_parameters window, which must contain at least one layer corresponding to the semi-infinite substrate ($t_N = \infty$). The total number of layers in the stratified medium is not limited.

1. A. Gibaud, X-ray and Neutron Reflectivity : Principles and Applications (Springer, Paris, 1999).

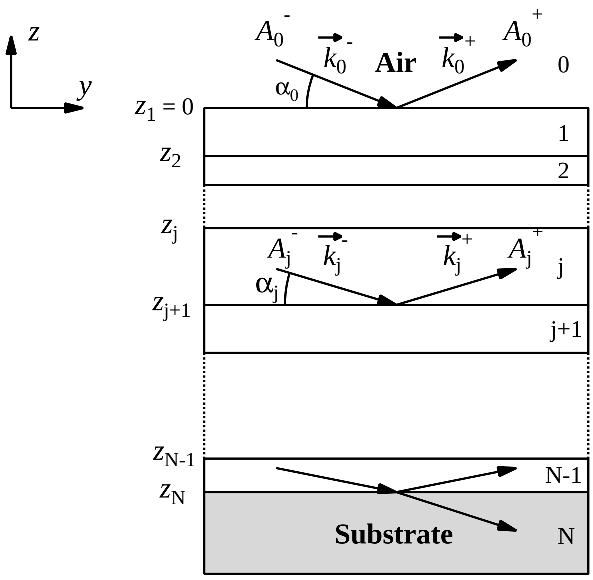

FIGURE 2 – Sketch of a plane wave propagating into a stratified medium. The z axis is perpendicular to the surface and its origin lies on the surface at $z_1 = 0$. The signs + (upward) and − (downward) label the direction of propagation of the wave.

It is possible to select the layer that contains the scattering objects by clicking the checkbox in front of the corresponding layer, which will appear with a green background color. In case of supported islands (*i.e.*, not included in a layer of the stratified medium), the upper checkbox will be automatically selected. *It is worth noting that only one 'scattering' layer can be selected.*

Sub-options of the Layer_parameters window

- Click the 'New table' button to create a new Layer_parameters table.
- Click the 'Display table' button to display the parameters in a standard Igor Pro table.
- Click the 'Insert layer' button to insert a new layer.
- Click the 'Delete layer' button to delete one layer.

4 GISAXS_parameters window

From the GISAXS_parameters window, you can define the model used to simulate the GISAXS data.

Layer geometry The following geometries are included in the FitGISAXS package :

- *Born approximation* : the GISAXS intensity is calculated within the Born approximation. Accordingly, refraction, reflection, and absorption effects are not taken into account in the calculation, and the parameters gathered in the 'Layer_parameter' window are not used.

– *Supported islands* : the form factor is calculated within the DWBA applied to a 2D assembly of islands supported on a substrate [2] (semi-infinite or stratified).

$$\begin{aligned} F\left(q_{\|}, k_{\mathrm{i,z}}, k_{\mathrm{f,z}}\right) &= F\left(q_{\|}, k_{\mathrm{f,z}} - k_{\mathrm{i,z}}\right) \\ &+ r_{0,1}\left(\alpha_{\mathrm{i}}\right) F\left(q_{\|}, k_{\mathrm{f,z}} + k_{\mathrm{i,z}}\right) \\ &+ r_{0,1}\left(\alpha_{\mathrm{f}}\right) F\left(q_{\|}, -k_{\mathrm{f,z}} - k_{\mathrm{i,z}}\right) \\ &+ r_{0,1}\left(\alpha_{\mathrm{i}}\right) r_{0,1}\left(\alpha_{\mathrm{f}}\right) F\left(q_{\|}, -k_{\mathrm{f,z}} + k_{\mathrm{i,z}}\right). \end{aligned}$$

– *Sandwiched islands* : the form factor is calculated within the DWBA applied to a 2D assembly of scatterers located at the interface z_{j+1} of a stratified medium [3].

$$\begin{aligned} F\left(q_{\|}, \widetilde{k}_{\mathrm{i,z}}, \widetilde{k}_{\mathrm{f,z}}\right) &= A_j^-\left(\alpha_{\mathrm{i}}\right) A_j^-\left(\alpha_{\mathrm{f}}\right) F\left(q_{\|}, \widetilde{k}_{\mathrm{f,z}} - \widetilde{k}_{\mathrm{i,z}}\right) \\ &+ A_j^+\left(\alpha_{\mathrm{i}}\right) A_j^-\left(\alpha_{\mathrm{f}}\right) F\left(q_{\|}, \widetilde{k}_{\mathrm{f,z}} + \widetilde{k}_{\mathrm{i,z}}\right) \\ &+ A_j^-\left(\alpha_{\mathrm{i}}\right) A_j^+\left(\alpha_{\mathrm{f}}\right) F\left(q_{\|}, -\widetilde{k}_{\mathrm{f,z}} - \widetilde{k}_{\mathrm{i,z}}\right) \\ &+ A_j^+\left(\alpha_{\mathrm{i}}\right) A_j^+\left(\alpha_{\mathrm{f}}\right) F\left(q_{\|}, -\widetilde{k}_{\mathrm{f,z}} + \widetilde{k}_{\mathrm{i,z}}\right), \end{aligned}$$

where A_j^+ and A_j^- are the complex amplitudes of the upward and downward propagating waves in layer j at the interface z_{j+1}.

– *Sandwiched layer* : the form factor is calculated within the DWBA applied to a 3D assembly of scatterers homogeneously distributed between the interface z_j and the interface z_{j+1} of a stratified medium [4].

$$\begin{aligned} \left|F\left(q_{\|}, q_{\mathrm{z}}\right)\right|^2 &= \left|A_j^-\left(\alpha_{\mathrm{i}}\right)\right|^2 \left|A_j^-\left(\alpha_{\mathrm{f}}\right)\right|^2 \left|F\left(q_{\|}, \widetilde{k}_{\mathrm{f,z}} - \widetilde{k}_{\mathrm{i,z}}\right)\right|^2 \frac{z_+}{t_j} \left[\exp\left(\frac{t_j}{z_+}\right) - 1\right] \\ &+ \left|A_j^+\left(\alpha_{\mathrm{i}}\right)\right|^2 \left|A_j^-\left(\alpha_{\mathrm{f}}\right)\right|^2 \left|F\left(q_{\|}, \widetilde{k}_{\mathrm{f,z}} + \widetilde{k}_{\mathrm{i,z}}\right)\right|^2 \frac{z_-}{t_j} \left[1 - \exp\left(-\frac{t_j}{z_-}\right)\right] \\ &+ \left|A_j^-\left(\alpha_{\mathrm{i}}\right)\right|^2 \left|A_j^+\left(\alpha_{\mathrm{f}}\right)\right|^2 \left|F\left(q_{\|}, -\widetilde{k}_{\mathrm{f,z}} - \widetilde{k}_{\mathrm{i,z}}\right)\right|^2 \frac{z_-}{t_j} \left[\exp\left(\frac{t_j}{z_-}\right) - 1\right] \\ &+ \left|A_j^+\left(\alpha_{\mathrm{i}}\right)\right|^2 \left|A_j^+\left(\alpha_{\mathrm{f}}\right)\right|^2 \left|F\left(q_{\|}, -\widetilde{k}_{\mathrm{f,z}} + \widetilde{k}_{\mathrm{i,z}}\right)\right|^2 \frac{z_+}{t_j} \left[1 - \exp\left(-\frac{t_j}{z_+}\right)\right], \end{aligned}$$

where $t_j = z_j - z_{j+1}$ is the thickness of the layer j, and $z_\pm$ can be expressed as a function of the penetration depth $z_{1/e}$ by

$$\frac{1}{z_\pm} = \frac{1}{z_{1/e}\left(\alpha_{\mathrm{i}}\right)} \pm \frac{1}{z_{1/e}\left(\alpha_{\mathrm{f}}\right)}.$$

2. M. Rauscher *et al.*, J. Appl. Phys. 86 (1999) 6763–6769.
3. S. Naranayan *et al.*, Phys. Rev. Lett. 94 (2005) 145504.
4. B. Lee *et al.*, Macromolecules 38 (2005) 3395–3405.

– *Buried layer* : the form factor is calculated within the DWBA applied to a 3D assembly of scatterers homogeneously distributed between the depths z_j and z_{j+1} of a semi-infinite medium [5]. This geometry is equivalent to the 'Sandwiched layer' geometry with the refractive indices of the different layers being equal to that of the substrate (*i.e.*, there is no upward propagating wave in the medium).

$$|F(\mathbf{q})|^2 = |t_{0,1}(\alpha_\mathrm{i})|^2 |t_{0,1}(\alpha_\mathrm{f})|^2 \frac{z_+}{t_j}\left[\exp\left(-\frac{z_j}{z_+}\right) - \exp\left(-\frac{z_{j+1}}{z_+}\right)\right] |F(\widetilde{\mathbf{q}})|^2 .$$

– *Correlated roughness* : the form factor is calculated within the DWBA by assuming that it originates from a 2D assembly of scatterers located at the interface z_{j+1} of a stratified medium and that their lateral positions are perfectly replicated to the surface roughness ($z_1 = 0$). Accordingly, the total scattered intensity is the sum of three terms describing (i) the intensity scattered by the objects located at the interface z_{j+1}, (ii) the intensity scattered by the objects located at the interface z_1, and (iii) the interference between them [6] :

$$|F(\mathbf{q})|^2 = |F_j(\mathbf{q})|^2 + |F_0(\mathbf{q})|^2 + 2\,|F_j(\mathbf{q})|\,|F_0(\mathbf{q})| \cos(q_\mathrm{z} z_{j+1}) ,$$

where $F_j(\mathbf{q})$ is the form factor of the buried scatterers and $F_0(\mathbf{q})$ is the form factor of the surface scatterers. Within this geometry, it is worth noting that the refractive index of the buried scatterers must be provided in the 'Fit_parameters' window. Furthermore, it is considered that the lateral (resp. vertical) size of the buried scatterers is proportional to the lateral (resp. vertical) size of the surface scatterers : *i.e.*, $D_0 = \xi_\mathrm{y} D_j$ and $H_0 = \xi_\mathrm{z} H_j$ where ξ_y (resp. ξ_z) characterizes the lateral (resp. vertical) correlation between the buried and surface scatterers.

– *Surface holes* : the form factor is calculated within the DWBA applied to a 2D assembly of holes located either on the top-layer (or substrate) surface ($z_1 = 0$) [7] or at the interface z_j of a stratified medium.

$$\begin{aligned} F\left(q_\parallel, \widetilde{k}_\mathrm{i,z}, \widetilde{k}_\mathrm{f,z}\right) \;=\;& B_j^-(\alpha_\mathrm{i})\, B_j^-(\alpha_\mathrm{f})\, F\left(q_\parallel, -\widetilde{k}_\mathrm{f,z} + \widetilde{k}_\mathrm{i,z}\right) \\ &+ B_j^+(\alpha_\mathrm{i})\, B_j^-(\alpha_\mathrm{f})\, F\left(q_\parallel, -\widetilde{k}_\mathrm{f,z} - \widetilde{k}_\mathrm{i,z}\right) \\ &+ B_j^-(\alpha_\mathrm{i})\, B_j^+(\alpha_\mathrm{f})\, F\left(q_\parallel, \widetilde{k}_\mathrm{f,z} + \widetilde{k}_\mathrm{i,z}\right) \\ &+ B_j^+(\alpha_\mathrm{i})\, B_j^+(\alpha_\mathrm{f})\, F\left(q_\parallel, \widetilde{k}_\mathrm{f,z} - \widetilde{k}_\mathrm{i,z}\right) , \end{aligned}$$

where B_j^+ and B_j^- are the complex amplitudes of the upward and downward propagating waves in layer j at the interface z_j.

5. D. Babonneau *et al.*, J. Appl. Crystallogr. 40 (2007) s350–s354.
6. D. Babonneau *et al.*, Phys. Rev. B 80 (2009) 155446.
7. N. Jedrecy *et al.*, Phys. Rev. B 72 (2005) 045430.

Form factor The following form factors are included in the FitGISAXS package (see Figs. 3 and 4) :

- *Spheroid* : in-plane diameter D_{y} and height H.
- *Random spheroid* : in-plane diameter D_{y} and height H (with random orientation).
- *Ellipsoid* : in-plane diameters D_{x}, D_{y}, and height H.
- *Cylinder* : in-plane diameter D_{y} and height H.
- *Hemispheroid* : in-plane diameter D_{y} and height H.
- *Truncated sphere* : in-plane diameter D_{y} and height H.
- *Facetted sphere* : in-plane diameter D_{y} and height H.
- *Capsule* : in-plane diameter D_{y} and height H.
- *Prism* : side D_{y} and height H.
- *Truncated tetrahedron* : side D_{y}, height H, and angle β.
- *Ripple1* : symmetric sinusoidal ripple with length D_{x}, width D_{y}, and height H.
- *Ripple2* : asymmetric sawtooth ripple with length D_{x}, width D_{y}, height H, and asymmetry factor A.
- *Anisotropic pyramid* : anisotropic pyramid with length D_{x}, width D_{y}, height H, and asymmetry factor A.
- *Core-shell spheroid* : core diameter D_{core}, core height H_{core}, and shell thickness t_{shell}.
- *Core-shell cylinder* : core diameter D_{core}, core height H_{core}, and shell thickness t_{shell} (the encapsulating shell is absent at the bottom of the core-shell cylinder).
- *Core-shell hemispheroid* : core diameter D_{core}, core height H_{core}, and shell thickness t_{shell} (the encapsulating shell is absent at the bottom of the core-shell
- *Core-shell ripple* : asymmetric sawtooth ripple covered with a shell (length D_{x}, width D_{y}, core height H_{core}, shell thickness t_{shell}, and asymmetry factor A).

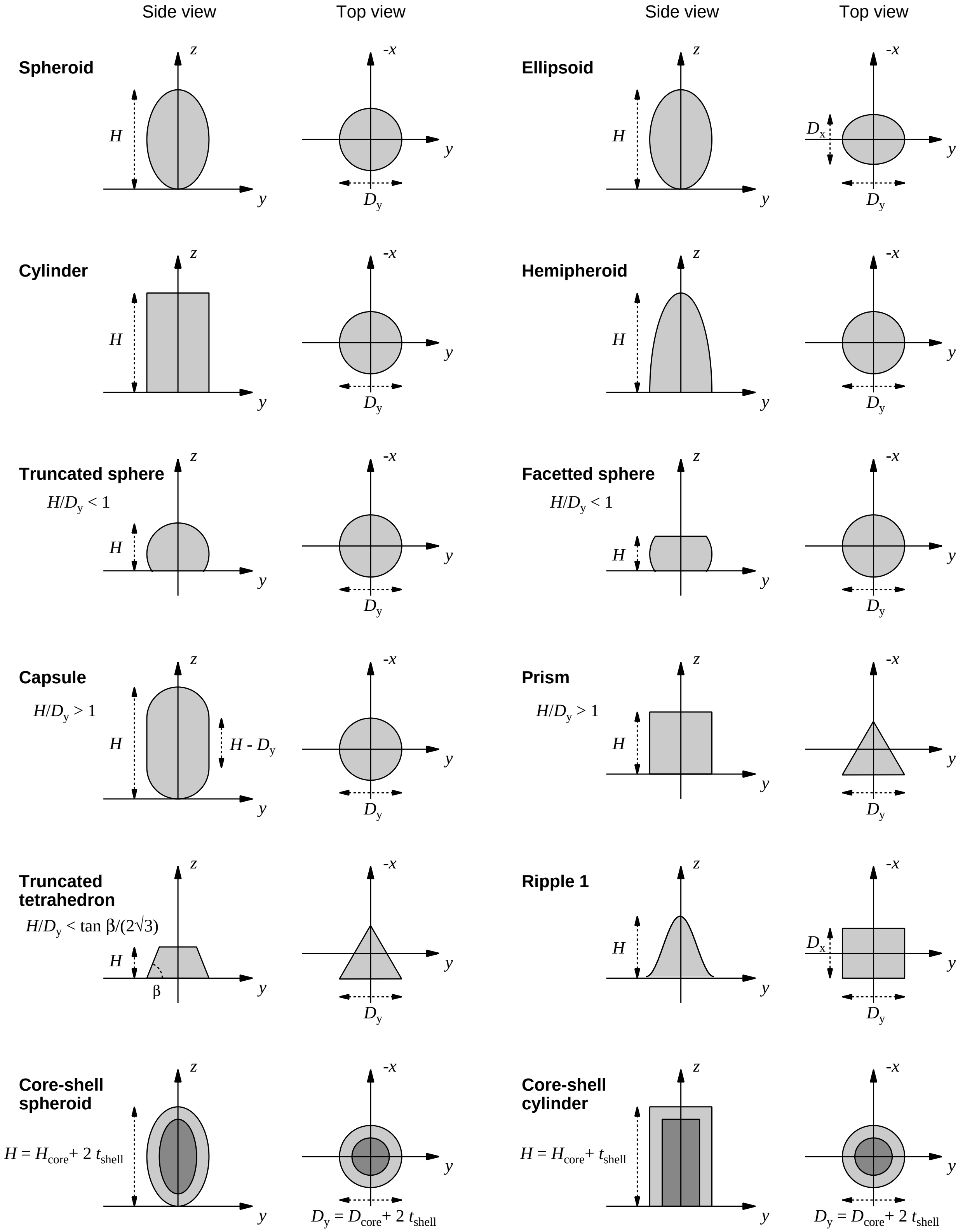

FIGURE 3 – Form factors included in the FitGISAXS package.

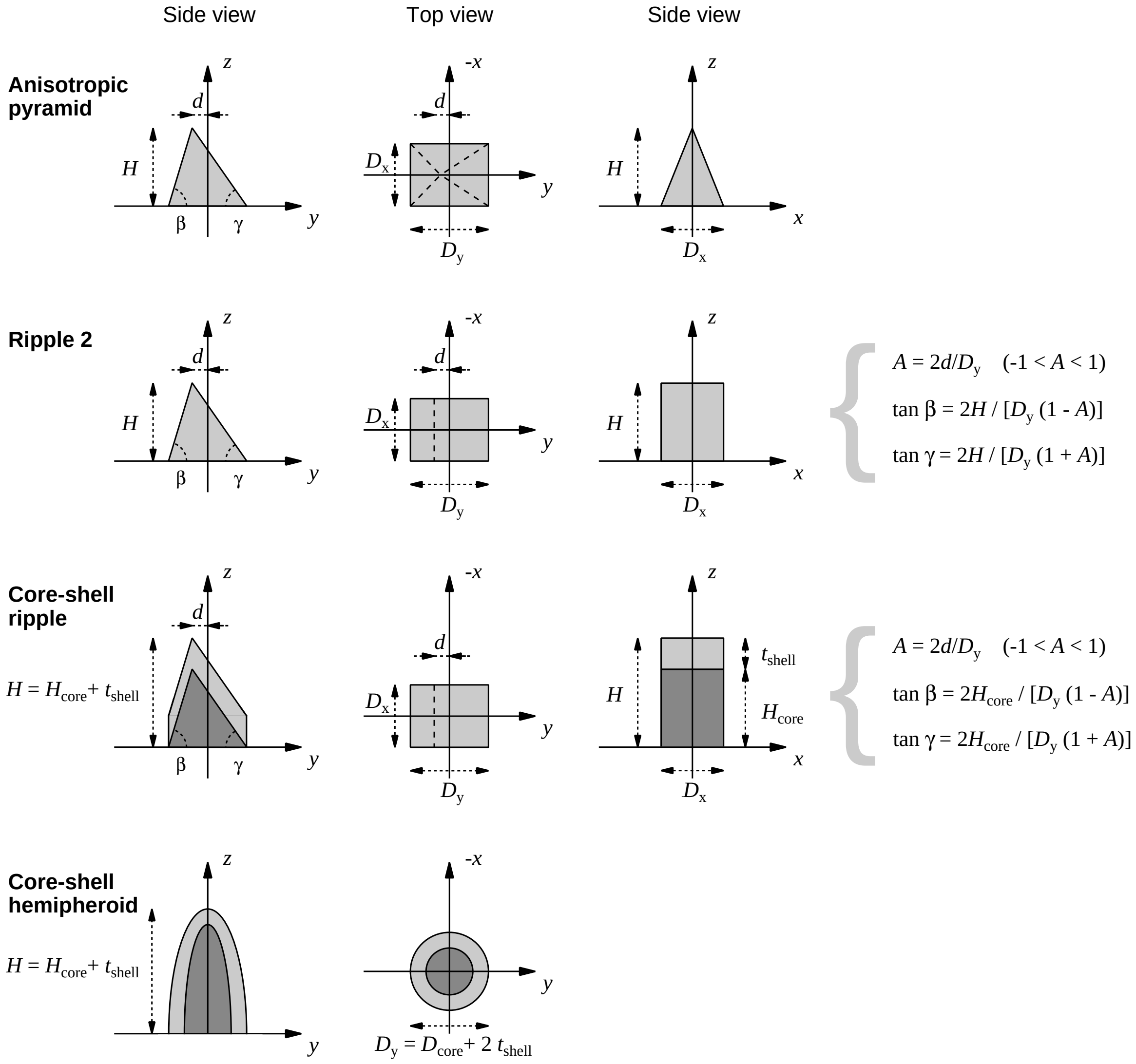

FIGURE 4 – Additional form factors included in the FitGISAXS package.

Structure factor The following structure factors are included in the FitGISAXS package :

- *Random organization* : $S(q) = 1$ with the scatterers being considered as isolated objects.
- *Percus-Yevick 3D* : the structure factor $S(q)$ is calculated *in the Born approximation* within the Percus-Yevick approximation for hard spheres with 3D short-range order. The hard-sphere diameter, D_{hs}, is assumed to be proportional to D_{y} with a constant factor C ($D_{\mathrm{hs}} = C \times D_{\mathrm{y}}$) and the hard-sphere volume fraction is η_{hs}.

$$S\left(q\right) = \left[1 + 24\frac{\eta_{\mathrm{hs}} G\left(qD_{\mathrm{hs}}\right)}{qD_{\mathrm{hs}}}\right]^{-1},$$

where

$$\begin{aligned} G(A) &= \alpha(\sin A - A\cos A)/A^2 + \beta[2A\sin A + (2-A^2)\cos A - 2]/A^3 \\ &+ \gamma\{-A^4\cos A + 4[(3A^2-6)\cos A + (A^3-6A)\sin A + 6]\}/A^5, \end{aligned}$$

and

$$\begin{aligned} \alpha &= (1+2\eta_{\mathrm{hs}})^2/(1-\eta_{\mathrm{hs}})^4 \\ \beta &= -6\eta_{\mathrm{hs}}(1+\eta_{\mathrm{hs}}/2)^2/(1-\eta_{\mathrm{hs}})^4 \\ \gamma &= \eta_{\mathrm{hs}}\alpha/2. \end{aligned}$$

- *Percus-Yevick 2D* : the structure factor $S(q_\parallel)$ is calculated within the Percus-Yevick approximation for hard spheres with 2D short-range order.

$$S\left(q_\parallel\right) = \left[1 + 24\frac{\eta_{\mathrm{hs}} G\left(q_\parallel D_{\mathrm{hs}}\right)}{q_\parallel D_{\mathrm{hs}}}\right]^{-1}.$$

- *Paracrystal 1D* : the structure factor $S(q_{\mathrm{y}})$ is calculated within the $1D$-paracrystal theory, while the scatterers are considered as isolated objects along the x-direction [Fig. 5(a)]. The mean interparticle distance, Λ_{y}, is assumed to be proportional to D_{y} with a constant factor C ($\Lambda_{\mathrm{y}} = C \times D_{\mathrm{y}}$) and the standard deviation is σ_{y}. Finite size effects can be introduced through a correlation length Λ_0 resulting in a broadening of the Dirac peak at $q_{\mathrm{y}} = 0$ (the Λ_0 value can be modified in the Structure_Paracrystal 1D.ipf procedure through the Windows\Procedure windows menu).

$$S\left(q_{\mathrm{y}}\right) = \frac{1 - \exp\left(-q_{\mathrm{y}}^2\sigma_{\mathrm{y}}^2\right)\exp\left(-2\frac{\Lambda_{\mathrm{y}}}{\Lambda_0}\right)}{1 - 2\exp\left(-\frac{1}{2}q_{\mathrm{y}}^2\sigma_{\mathrm{y}}^2\right)\exp\left(-\frac{\Lambda_{\mathrm{y}}}{\Lambda_0}\right)\cos\left(q_{\mathrm{y}}\Lambda_{\mathrm{y}}\right) + \exp\left(-q_{\mathrm{y}}^2\sigma_{\mathrm{y}}^2\right)\exp\left(-2\frac{\Lambda_{\mathrm{y}}}{\Lambda_0}\right)}.$$

- *Paracrystal 2D-rec* : the structure factor $S(q_\parallel)$ is calculated within the $2D$-paracrystal theory assuming a rectangular lattice [Fig. 5(b)]. The mean lattice parameters along the x- and y-directions are Λ_{x} and Λ_{y}, respectively, with $\Lambda_{\mathrm{y}} = C \times D_{\mathrm{y}}$ and with $\Lambda_{\mathrm{x}} \propto \Lambda_{\mathrm{y}}$. The corresponding standard deviations are σ_{x} and σ_{y}.

$$S\left(q_\parallel\right) = \prod_{k=\mathrm{x,y}} \frac{1 - \exp\left(-q_\parallel^2\sigma_k^2\right)\exp\left(-2\frac{\Lambda_k}{\Lambda_0}\right)}{1 - 2\exp\left(-\frac{1}{2}q_\parallel^2\sigma_k^2\right)\exp\left(-\frac{\Lambda_k}{\Lambda_0}\right)\cos\left(q_k\Lambda_k\right) + \exp\left(-q_\parallel^2\sigma_k^2\right)\exp\left(-2\frac{\Lambda_k}{\Lambda_0}\right)}.$$

- *Paracrystal 2D-hex* : the structure factor $S(q_\parallel)$ is calculated within the $2D$-paracrystal theory assuming an hexagonal lattice [Fig. 5(c)]. The mean lattice parameter, Λ_{y}, is

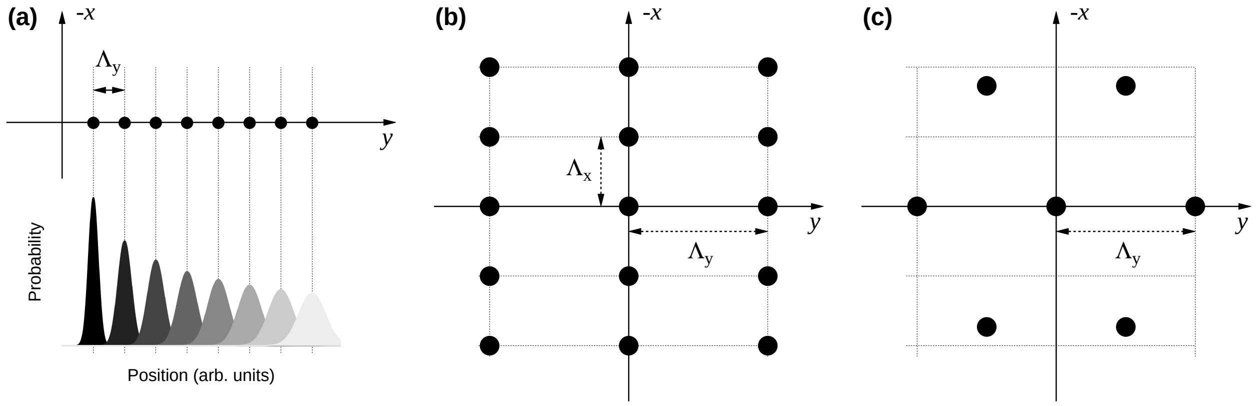

FIGURE 5 – (a) $1D$-paracrystal model with cumulative gaussian disorder resulting in a loss of long range order. (b) $2D$-paracrystal model with rectangular lattice. (c) $2D$-paracrystal model with hexagonal lattice.

assumed to be proportional to D_y with a constant factor C ($\Lambda_y = C \times D_y$) and the standard deviation is σ_y.

$$S\left(q_{\|}\right) = \prod_{k=\mathrm{x,y}} \frac{1-\exp\left(-q_{\|}^2\sigma_y^2\right)\exp\left(-2\frac{\Lambda_y}{\Lambda_0}\right)}{1-2\exp\left(-\frac{1}{2}q_{\|}^2\sigma_y^2\right)\exp\left(-\frac{\Lambda_y}{\Lambda_0}\right)\phi_k+\exp\left(-q_{\|}^2\sigma_y^2\right)\exp\left(-2\frac{\Lambda_y}{\Lambda_0}\right)},$$

where $\phi_x = \cos\left(q_x\Lambda_y\sqrt{3}/2 + q_y\Lambda_y/2\right)$ and $\phi_y = \cos\left(q_y\Lambda_y\right)$. It should be noted that the sixfold symmetry might be restored by calculating an average value of the interference function after successive rotations of 60° (see the Structure_Paracrystal 2D-hex.ipf procedure through the Windows\Procedure windows menu).

Size distribution model The GISAXS data can be calculated within the *monodisperse approximation* (MA), the *local monodisperse approximation* (LMA), and the *decoupling approximation* (DA) [8]. It is worth noting that the DA cannot be applied to the 'Sandwiched layer', 'Buried layer', and 'Correlated roughness' geometries.

Distribution function The following size-distribution functions $N(D)$ calculated between $D_{\min}$ and $D_{\max}$ are included in the FitGISAXS package :

– *Gaussian* : mean diameter D and full width at half-maximum $FWHM$,

$$N(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{(x-D)^2}{2\sigma^2}\right],$$

where

$$\sigma = \frac{FWHM}{2\sqrt{2\ln 2}}.$$

8. J. S. Pedersen *et al.*, J. Appl. Crystallogr. 27 (1994) 595–608.

- *DoubleGaussian* : bimodal gaussian distribution with mean diameters D and D_2 and full widths at half-maximum $FWHM$ and $FWHM_2$.
- *Log-normal* : mean of the diameter logarithm $\ln D$ and full width at half-maximum $FWHM$,

$$N(x) = \frac{1}{x \ln \sigma \sqrt{2\pi}} \exp\left[-\frac{1}{2}\frac{(\ln x - \ln D)^2}{(\ln \sigma)^2}\right],$$

where

$$\ln \sigma = \frac{1}{\sqrt{2 \ln 2}} \operatorname{asinh}\left(\frac{FWHM}{2D}\right).$$

The average diameter D_{avg} and the maximum of the distribution $D_{\max}$ are related to D and $\ln \sigma$ by

$$D_{\text{avg}} = D \exp\left[\frac{1}{2}(\ln \sigma)^2\right],$$

and

$$D_{\max} = D \exp\left[-(\ln \sigma)^2\right].$$

- *DoubleLog-normal* : bimodal log-normal distribution with mean of the diameters logarithm $\ln D$ and $\ln D_2$ and full widths at half-maximum $FWHM$ and $FWHM_2$.
- *Weibull* : scale parameter D and shape parameter $FWHM$,

$$N(x) = \frac{FWHM}{D}\left(\frac{x}{D}\right)^{FWHM-1} \exp\left[-\left(\frac{x}{D}\right)^{FWHM}\right]. \tag{1}$$

H/D In many cases, a correlation between the in-plane size D and the height H of the scatterers exists so that D and H cannot be decoupled in the fitting process. The following correlations are included in the FitGISAXS package :
- *Constant* : $H/D = C_1$.
- *Polynomial* : $H/D = C_2 \times (C_1 + 1/D)$. $C_1 = 0$ implies that H is a constant equal to C_2.

5 Fit_parameters window

The Fit_parameters window contains all the fitting parameters ('Fitting parameters' tab) and other fixed parameters ('More parameters' tab) such as the wavelength of the incident X-ray beam, the angle of incidence, the azimuthal angle (in-plane rotation about the z-axis), and the tilt angle (out-of-plane rotation about the x-axis). It should be noted that the tilt angle cannot be applied to the 'Capsule', 'Prism', 'truncated tetrahedron', 'Ripple1', 'Ripple2', and 'Core-shell ripple' form factors. The refractive index (*i.e.*, δ and β values) of the scattering objects ('scatterers') or of the core-shell particles ('core' and 'shell') can be also entered in this window.

6 FitGISAXS menu

The FitGISAXS menu has several options :

Load GISAXS...

Click the 'Load GISAXS...' option to plot 2D experimental GISAXS data. Different data format are supported, including tiff image file ('Image file' sub-option) and matrix from text file ('Text file' sub-option). However, if your data format is not supported by the FitGISAXS package, please email me (mailto : david.babonneau@univ-poitiers.fr). Once the 'Enter parameters' dialog has appeared, you must provide the angle of incidence, the azimuthal angle, the lateral and vertical positions of the direct beam, the sample-to-detector distance, and the energy of the incident X-ray beam (see Fig. 6).

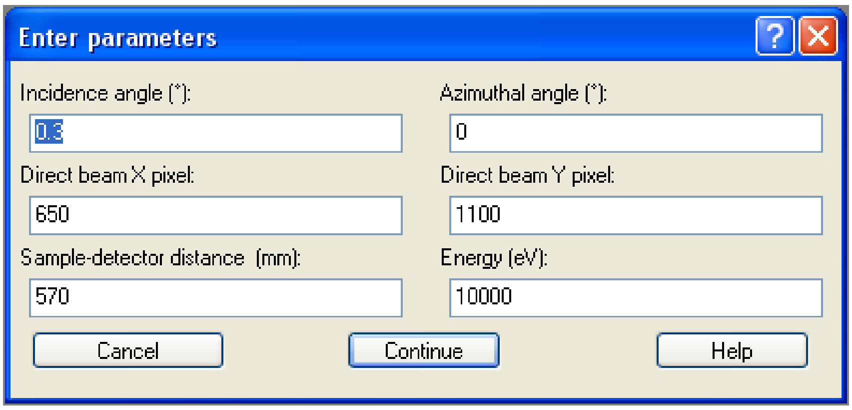

FIGURE 6 – A screen shot of the 'Load GISAXS...' dialog.

By default, the experimental data are plotted in linear intensity scale as a function of the in-plane ($2\theta_f$) and out-of-plane (α_f) angles in emergence (see Fig. 7). The intensity scale of the image (min. and max. intensity values) can be adapted in the upper-left corner of the window.

- Click the '1/nm' (resp. 'deg') button to display the data as a function of $q_y = 2\pi[\sin(2\theta_f)]/\lambda$ and $q_z = 2\pi[\sin(\alpha_f) + \sin(\alpha_i)]/\lambda$ (resp. $2\theta_f$ and α_f).

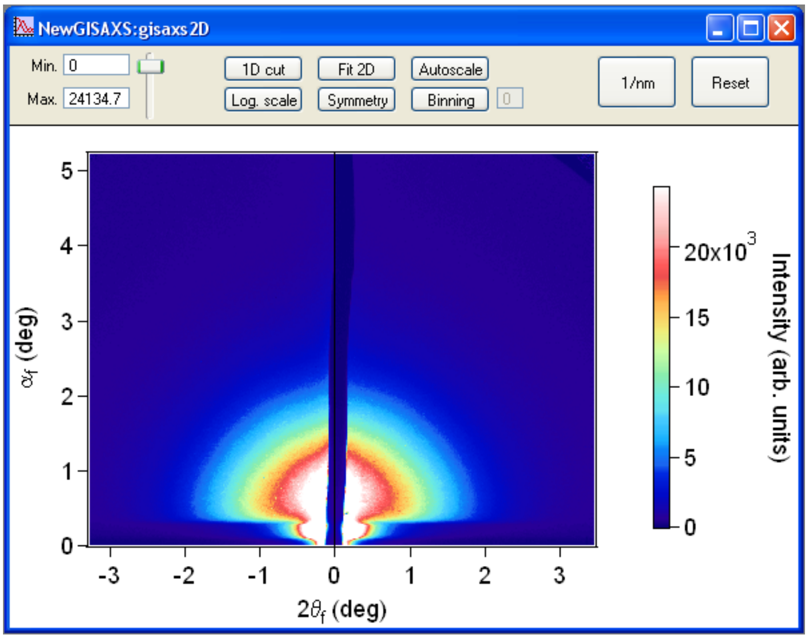

Figure 7 – 2D experimental GISAXS data as displayed by using the 'Load GISAXS...' option.

– The data values can be logarithmically (resp. linearly) mapped by clicking the 'Log. scale' (resp. 'Lin. scale') button.

– Click the 'Symmetry' button to obtain a symmetric image, *i.e.* $I(2\theta_f) = I(-2\theta_f)$ or $I(q_y) = I(-q_y)$.

– Click the 'Binning' button to merge the pixels 2×2.

– Click the 'Autoscale' button to perform a full range scaling of the horizontal and vertical axes.

– Click the 'Reset' button to cancel all the previous operations.

– Click the '1D cut' button to plot a 1D cut of the image. This option is available only when the data are plotted in linear intensity scale as a function of $2\theta_f$ and α_f. The '1D cut' operation opens a dialog window in which you can enter the cut *angle* (0 for a cut parallel to the $2\theta_f$ axis, 90 for a cut parallel to the α_f axis, or any other value in the range between 0 and 90), the cut *position* (*i.e.*, the α_f position if *angle* is 0 or the $2\theta_f$ position if *angle* is 90 ; by default, the cut position is 0 if *angle* is different from 0 or 90), and the cut *width* (*i.e.*, the 1D data are averaged from $position - width/2$ to $position + width/2$ if $angle = 0$ or 90, or from $angle - width/2$ to $angle + width/2$ if

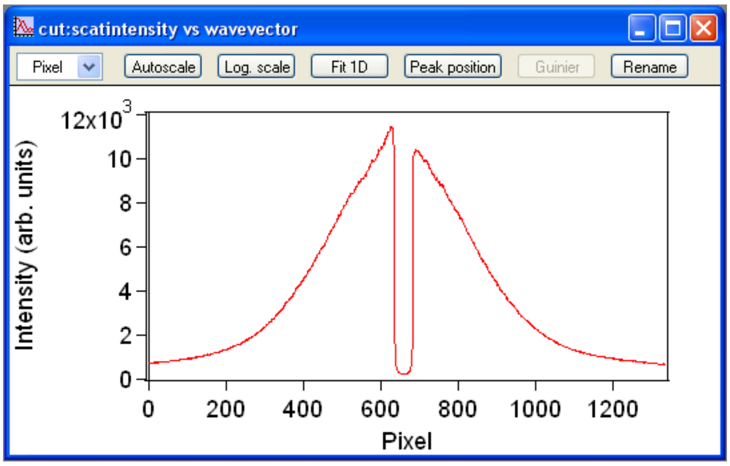

FIGURE 8 – 1D experimental GISAXS data as displayed by using the '1D cut' button.

angle is different from 0 or 90). Once the 'continue' button has been clicked, red lines delimiting the integrated area appear on the 2D image and 1D data are plotted in a new 'cut' window (see Fig. 8).

By default, the 1D data are named *scatintensity* vs *wavevector*, but they can be renamed by clicking the 'rename' button (upper-right corner of the 'cut' window). Moreover, the 1D data are plotted as a function of the pixel value, but they can be also plotted as a function of $2\theta_f$, α_f, $q_\mathrm{x} = 2\pi[\cos(2\theta_f)\cos(\alpha_f) - \cos(\alpha_i)]/\lambda$, $q_\mathrm{y} = 2\pi[\sin(2\theta_f)\cos(\alpha_f)]/\lambda$, or $q_\mathrm{z} = 2\pi[\sin(\alpha_f) + \sin(\alpha_i)]/\lambda$ (upper-left corner of the 'cut' window).

If an interference maximum is present on the curve, it is possible to determine its position by placing the cursor A (resp. B) before (resp. after) the maximum and by clicking the 'Peak position' button. The result is then printed in the command window. If the data are plotted in q-scale, it is also possible to click the 'Guinier' button in order to plot the corresponding $\ln I(q)$ vs q^2 curve, which appears in a new 'Guinier_plot' window. Then, by placing cursors A and B on the curve and by clicking the 'Diameter' button, a linear fit is performed and the slope s is printed in the command window as well as the Guinier diameter $D_g = 2\sqrt{-3s}$, and the corresponding diameter $D = D_g\sqrt{5/3}$ assuming spherical scatterers.

If the data are plotted as a function of the pixel value, you can click the '1D fit' button to open a new 'Fit1D_parameters' window, which contains a list of the fitting parameters. Then, you can modify the parameters and click the 'Plot now' button to plot 1D calculated data in the 'cut' window. After having placed the cursors A and B over a convenient range, you can also click the 'Fit now' button to fit the 1D experimental data. If you want to hold a parameter while fitting then tick the checkbox. If left unchecked then the parameter will vary in the fitting process, and it will be updated in the Fit_parameters window.

– After having placed the cursors A and B in the 'NewGISAXS' window, click the '2D fit' button to select a part of the image delimited by A (lower-left corner) and B (upper-right corner). This option is available only when the data are plotted in linear intensity scale as a function of $2\theta_f$ and α_f. The '2D fit' operation opens a new 'cut2d' window (which displays the selected part of the image) and a new 'Fit2D_parameters' window (which contains a list of the fitting parameters). Then, you can modify the parameters and click the 'Plot now' button to plot 2D calculated data or the 'Fit now' button to fit the 2D experimental data. In both cases, the calculated/fitted data are plotted in a new 'Fit_gisaxs2D' window and the residual data (experimental data − calculated/fitted data) are plotted in a new 'Res_gisaxs2D' window. It is also worth noting that, depending on the complexity of the model, both the plotting process and the fitting process may take a long time. Therefore, it is strongly recommended to select a small image area or to use the 'binning' option, and to hold a maximum of parameters.

Create GISAXS...

Click the 'Create GISAXS...' option to plot 2D calculated GISAXS maps ($Q_\mathrm{y}, Q_\mathrm{z}$ map at fixed Q_x, $Q_\mathrm{x}, Q_\mathrm{z}$ map at fixed Q_y, $Q_\mathrm{x}, Q_\mathrm{y}$ map at fixed Q_z) or 1D GISAXS curves (Q_y cut at fixed Q_x and Q_z, Q_z cut at fixed Q_x and Q_y). *It is worth noting that the Ewald sphere curvature is not taken into consideration in the calculations when using the 'Create GISAXS...' option.*

Once the GISAXS intensity have been calculated and displayed, then the input parameters can be modified in the GISAXS_parameters and Fit_parameters windows, and the data can be updated by clicking the 'Update' button. From 1D GISAXS curves, it is also possible to click the 'Guinier' button in order to plot the corresponding $\ln I(q)$ vs q^2 curve.

Layer parameters...

Click the 'Layer parameters...' option to display/update the Layer_parameters window.

GISAXS parameters...

Click the 'GISAXS parameters...' option to display/update the GISAXS_parameters window.

Fit parameters...

Click the 'Fit parameters...' option to display/update the Fit_parameters window.

Plot form factor...

Click the 'Plot form factor...' option to plot the 1D form factor of the scatterers within the Born approximation and the monodisperse approximation : both $|F(q_{\mathrm{y}}, q_{\mathrm{z}} = 0)|^2$ and $|F(q_{\mathrm{y}} = 0, q_{\mathrm{z}})|^2$ are plotted.

Plot structure factor...

Click the 'Plot structure factor...' option to plot the 1D structure factor of the assembly within the Born approximation and the monodisperse approximation : both $S(q_{\mathrm{y}}, q_{\mathrm{z}} = 0)$ and $S(q_{\mathrm{y}} = 0, q_{\mathrm{z}})$ are plotted. It is possible to determine the position of the interference maximum by positioning the cursor A (resp. B) over the plotted curves before (resp. after) the maximum and by clicking the 'Peak position' button. The result is then printed in the command window.

Plot size distribution...

Click the 'Plot size distribution...' option to plot the size distribution of the scatterers (D and H) between D_{min} and D_{max}. This option is not available when the 'Monodisperse approximation' size distribution model is selected in the GISAXS_parameters window.

Plot shape distribution...

Click the 'Plot shape distribution...' option to plot the correlation between H and D, and between H/D and D in the $D_{\mathrm{min}} - D_{\mathrm{max}}$ range. This option is not available when the 'Monodisperse approximation' size distribution model is selected in the GISAXS_parameters window.

Plot reflection...

Click the 'Plot reflection...' option to plot the reflectivity of the stratified medium described in the Layer_parameters window (*i.e.*, $|A_0^+|^2/|A_0^-|^2$).

Plot transmission...

Click the 'Plot transmission...' option to plot the transmission coefficient of the layer $\sharp 1$ of the stratified medium (or the substrate) described in the Layer_parameters window.

Penetration depth...

Click the 'Penetration depth...' option to plot the penetration depth of the layer $\sharp 1$ of the stratified medium (or the substrate) described in the Layer_parameters window.

Plot EFI...

Click the 'Plot EFI...' option to plot the electric field intensity (EFI) distribution of the stratified medium described in the Layer_parameters window.

- *EFI 1D vs depth* : Plot the EFI as a function of the depth at a fixed angle of incidence.
- *EFI 1D vs angle* : Plot the EFI as a function of the angle of incidence at a fixed depth.
- *EFI 2D* : Plot the EFI as a function of the angle of incidence and depth.
- U_- : Plot the intensity of the downward propagating wave as a function of the angle of incidence in layer j at the interface z_{j+1}.
- U_+ : Plot the intensity of the upward propagating wave as a function of the angle of incidence in layer j at the interface z_{j+1}.
- V_- : Plot the intensity of the downward propagating wave as a function of the angle of incidence in layer $j+1$ at the interface z_{j+1}.
- V_+ : Plot the intensity of the upward propagating wave as a function of the angle of incidence in layer $j+1$ at the interface z_{j+1}.

7 Forthcoming developments

FitGISAXS is still under development. Among the future improvements, the full description within the DWBA of the structure factor using the paracrystal 3D model for self-organized multilayers [9] is forecasted.

If you have any suggestions on how to improve things or if you would like to help develop things then please email me (mailto : `david.babonneau@univ-poitiers.fr`).

8 Bugs

I disclaim any problems, which could result from the use of the program. Send me details of any bugs and I will try to fix them.

9 Acknowledging the use of FitGISAXS

If you use FitGISAXS to analyse data that you then use in a publication, please acknowledge the use of FitGISAXS by citing the reference :

***FitGISAXS : software package for modelling and analysis of GISAXS data using IGOR Pro,* D. Babonneau, J. Appl. Crystallogr. 43 (2010) 929–936.**

9. M. Buljan *et al.*, Acta Cryst. A 68 (2012) 124–138.