On the instrumental resolution in X-ray reflectivity experiments

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A general method to describe the instrumental resolution function for grazing-angle X-ray scattering experiments is presented. A resolution function $R$ is introduced as the Gaussian joint-distribution function of the (interdependent) random deviation $\mathbf{q}'$ associated with the wavevector transfer $\mathbf{q}$. Useful expressions for the mean square values of $\mathbf{q}'$ are derived for some common scattering geometries, such as rocking scans, and scans out of the plane of incidence. The mean square values related to the incident beam dispersion and the detector acceptance angles are included in the treatment of $R$. As an example, $R$ is incorporated in the calculation of the diffuse scattering from freestanding smectic films within the framework of the first Born approximation and the main resolution effects are discussed.

1. Introduction

Grazing-angle X-ray scattering is being extensively used to study the structure and interfacial properties of hard and soft thin films. As an example, X-ray reflectivity and surface diffraction are powerful techniques to probe normal and in-plane structures on the molecular scale (e.g. Holý et al., 1999), and X-ray diffuse scattering has been shown to be very useful in determining the interfacial properties of thin liquid films, such as the surface tension and bending elasticity modulus (e.g. Gompper & Schick, 1994; Tolan, 1999). In all these experiments, the experimental resolution must be carefully taken into account as the physical information is intimately mixed up with it. The origin of the resolution stems from the properties of the particular scattering geometry pictured in Fig. 1 for a $z$-axis setup. The vector $\mathbf{k}_{\text{in}}$ defines the direction of the beam incident on the sample; the plane defined by the $(Oz)$ axis and $\mathbf{k}_{\text{in}}$ is called the plane of incidence. The direction of $\mathbf{k}_{\text{in}}$ is experimentally defined by $\alpha_i$ and $\alpha_o$. The incident beam has in general a rectangular cross section defined by two orthogonal sets of slits $S_E$ and $S_F$ perpendicular to $\mathbf{k}_{\text{in}}$ (preshape slits). The scattered vector $\mathbf{k}_{\text{out}}$ is defined by the position of the detector at the angles $\beta_i$ and $\beta_o$; the plane defined by $\mathbf{k}_{\text{in}}$ and $\mathbf{k}_{\text{out}}$ is called the scattering plane. The detector entrance is defined by two orthogonal sets of slits $S_D$ and $S_D'$ perpendicular to $\mathbf{k}_{\text{out}}$. The experimental resolution includes the wavelength dispersion, the beam angular divergence and the detector acceptance angles. In other words, $\mathbf{k}_{\text{in}}$ and $\mathbf{k}_{\text{out}}$ are not ideally defined, but dispersed. The dispersion relative to $\mathbf{k}_{\text{in}}$ depends on the optical setup before the sample (source, monochromator etc.). The dispersion relative to $\mathbf{k}_{\text{out}}$ comes from purely geometrical considerations. It is due to the existence of acceptance angles as defined by the detector slits and the illuminated area on the sample (footprint). The measured scattered intensity $I$ results from averaging over the angular deviations and can be expressed as a function the wavevector transfer $\mathbf{q} = \mathbf{k}_{\text{out}} - \mathbf{k}_{\text{in}}$. It can be written as the convolution of the scattering function $S(\mathbf{q})$ with a resolution function $R$ describing the distribution of the deviations $\mathbf{q}'$ around $\mathbf{q}$:

$$I(\mathbf{q}) = \int S(\mathbf{q} - \mathbf{q}')R(\mathbf{q}')\,d\mathbf{q}'$$

Figure 1
General scattering geometry of a $z$-axis (vertical) setup. The incidence plane is defined by the incident wavevector $\mathbf{k}_i$ and the surface normal $(Oz)$; the scattering plane is defined by the scattered wavevector $\mathbf{k}_o$ and $\mathbf{k}_{\text{in}}$.

This formalism is appealing because it allows the advantageous use of the reciprocal-space representation of the scattering function $S(\mathbf{q})$. For instance, in the first Born approximation, $S$ is simply given by the Fourier transform of the density–density correlation function:

$$S(\mathbf{q}) = \int d^3r \exp(i\mathbf{q} \cdot \mathbf{r})\rho(0)\rho(\mathbf{r})$$

Note that equation (1) is valid only in the incoherent limit. The effects of partial coherence have their importance especially...
when using synchrotron radiation and have been discussed elsewhere (Sinha et al., 1998; Bernhoeft et al., 1998).

So far, calculations of \( \beta \) have been limited to specific situations, such as specular reflectivity (Gibaud et al., 1993), detector scans in the plane of incidence (de Juë et al., 1996) and Bragg diffraction (Höfle et al., 1999). In these geometries the incident and the scattering plane coincide and equation (1) boils down to simply averaging the scattering function over a resolution area in the plane of incidence. More complicated scattering geometries associated with surface diffraction (Vlieg, 1997) or scattering out of the plane of incidence (Mol et al., 1997) require averaging over a full resolution volume. In such situations, \( \beta \) has not always been clearly analyzed. The aim of this paper is to present a general method to calculate \( \beta \).

In §2, we derive a general form for the resolution function, taking into account the deviations associated with the beam dispersion and the detector acceptance angles. In §3, useful expressions relating reciprocal- and direct-space mean square deviations are derived for some common scattering geometries. In §4, a suitable method is given to determine the mean square values of the experimental parameters. Finally, in §5, we discuss the effect of the resolution on the particular example of scattering from free-standing smectic films.

2. General resolution function

Let us start with the description of dispersions relative to \( \mathbf{k}_{\text{in}} \) and \( \mathbf{k}_{\text{out}} \) by introducing random deviations \( \alpha_{\text{i, o}} \) and \( \beta_{\text{i, o}} \) around the angles \( \alpha_{\text{i, o}} \) and \( \beta_{\text{i, o}} \), respectively. In what follows we assume that \( \alpha_{\text{i, o}} \) and \( \beta_{\text{i, o}} \) can be described by a Gaussian distribution and are statistically independent. In this case they are fully described by their mean square deviations \( \Delta \alpha_{\text{i, o}}^2 = \langle (\alpha_{\text{i, o}})^2 \rangle \) and \( \Delta \beta_{\text{i, o}}^2 = \langle (\beta_{\text{i, o}})^2 \rangle \). Furthermore, we assume the random deviations to be small. This allows use of a linear relation between the angular deviations and \( \mathbf{q} \). From Fig. 1, the relation between \( \mathbf{q} \) and the four angles is

\[
\begin{align*}
q_x &= k(\cos \beta \sin \alpha - \cos \alpha \sin \beta), \\
q_y &= k(\cos \beta \sin \alpha + \cos \alpha \sin \beta), \\
q_z &= k(\sin \alpha + \sin \beta),
\end{align*}
\]

where \( k = 2\pi/\lambda \) and \( \lambda \) is the wavelength. For the sake of simplicity, we assume the beam to be ideally monochromated, so that we can disregard the wavelength dispersion \( \Delta \lambda \). After taking the partial derivatives, we obtain

\[
\begin{align*}
q'_x &= k(\alpha' \sin \alpha \cos \alpha + \alpha' \cos \alpha \sin \alpha - \beta' \sin \beta \cos \beta - \beta' \cos \beta \sin \beta), \\
q'_y &= k(-\alpha' \sin \alpha \cos \alpha - \alpha' \cos \alpha \sin \alpha + \beta' \sin \beta \cos \beta + \beta' \cos \beta \sin \beta), \\
q'_z &= k(\alpha' \cos \alpha + \beta' \cos \beta).
\end{align*}
\]

These linear relations together with mean square deviations \( \Delta \alpha_{\text{i, o}}^2 \) and \( \Delta \beta_{\text{i, o}}^2 \) allow us to write down the mean square deviations of \( \mathbf{q} \):

\[
\langle q'_i, q'_j \rangle = k^2(\sin^2 \alpha \cos^2 \alpha \Delta \alpha_i^2 + \cos^2 \alpha \sin^2 \alpha \Delta \alpha_i^2
+ \sin^2 \beta \cos^2 \beta \Delta \beta_i^2 + \cos^2 \beta \sin^2 \beta \Delta \beta_i^2),
\]

\[
\langle q'_i, q'_j \rangle = k^2(\sin^2 \alpha \sin^2 \alpha \Delta \alpha_i^2 + \cos^2 \alpha \cos^2 \alpha \Delta \alpha_i^2
+ \sin^2 \beta \sin^2 \beta \Delta \beta_i^2 + \cos^2 \beta \cos^2 \beta \Delta \beta_i^2).
\]

The general resolution function \( \overline{r}(\mathbf{q}) \), defined as the Gaussian joint-distribution function of the random deviations \( q'_i, q'_j, q'_z \), is expressed as follows (e.g. van Kampen, 1981):

\[
\overline{r}(\mathbf{q}) = [\det A^{-1}/(2\pi)^{3/2}] \exp(-1/2 \mathbf{q} \cdot A^{-1} \mathbf{q}),
\]

where \( A = \langle q'_i q'_j \rangle \) is the covariance matrix of the random deviation \( \mathbf{q} \) as given by equation (5). The prefactor in equation (6) is simply a normalization factor. From here on, we assign the eigenvalues of \( A \) to be \( \Delta q_{\|}^2, \Delta q_{\perp}^2 \) and \( \Delta q_z^2 \), and let \((\Omega, x, y, z)\) refer implicitly to the eigenvector coordinate system of \( A \). Then the analytical convolution in equation (1) in combination with equation (2) leads to the following general expression for the intensity:

\[
I = \int d^3 r \exp[\mathbf{q} \cdot r - (1/2)x^2 \Delta q_{\|}^2 - (1/2)y^2 \Delta q_{\perp}^2
- (1/2)z^2 \Delta q_z^2] \rho(0) \rho(r).
\]

The next step consists of carrying out the integration in equation (7). We will describe how to perform this integration in the case of diffuse scattering from free-standing smectic films in §5. The relation between the reciprocal- and direct-space mean square deviations is not straightforward. In the next section, we shall give some useful approximations for some common scattering geometries, such as rocking scans and diffuse scans out of the plane of incidence.

3. Application to specific scattering geometries

Let us consider first scattering geometries where \( \mathbf{q} \) stays in the plane of incidence \( (q_z = 0, \alpha_o = \beta_o = 0) \). This is, for example, the case for so-called rocking scans (see Fig. 2) where \( \omega = (\alpha_i - \beta_i)/2 \) is varied, while \( \theta = (\alpha_i + \beta_i)/2 \) is kept constant. In this case \( q_z \) is varied while \( q_z \) is kept effectively almost constant over the accessible range determined by the constraint \( |\omega| \leq \theta \). It also applies to detector scans in the plane of incidence, for which \( \beta_i \) is varied while \( \alpha_i \) is kept constant (Daillant et al.,...
$$I(q_x, q_z) = \int dq_x' \int dq_z' \mathcal{R}(q_x', q_z') S(q_x - q_x', q_z - q_z'),$$  \hspace{1cm} (10)$$

but with \( \mathcal{R} \) and \( S \) defined as

$$\mathcal{R}(q_x, q_z) = (1/2\pi\Delta q_x\Delta q_z) \exp[-(q_x^2/2\Delta q_x^2) - (q_z^2/2\Delta q_z^2)]$$

and

$$S(q_x, q_z) = [(2\pi)^{1/2}/\Delta q_z] \int dq_x \exp(iq_x x + iq_z z) \times \langle \rho(0)\rho(x, y = 0, z) \rangle.$$

Now, let us consider the case of detector scans out of the plane of incidence, which are extensively used in solid-state surface diffraction experiments (Vlieg, 1997), and in diffuse scattering experiments on liquid surfaces (Mol et al., 1997; Daillant et al., 1996). As shown in Fig. 3, in this situation the detector is moved by an angle \( \beta_0 \) while \( \alpha_0 = 0 \). To optimize the diffuse signal, \( \alpha_0 = \beta_0 \) is often used in addition. In this way, \( q_x \) and \( q_z \) are probed over a large and small range, respectively, while \( q_y \) is kept constant on the specular ridge, as deduced from equation (3). In this geometry, the scattering cross section is limited by the resolution in all directions in space. From equation (5), and keeping only leading order terms, \( A \) reads:

$$A/k^2 = \begin{bmatrix} \alpha_x^2\Delta \alpha_x^2 + \beta_x^2\Delta \beta_x^2 & 0 & \alpha_x\Delta \alpha_x^2 - \beta_x\Delta \beta_x^2 \\ 0 & \Delta \alpha_x^2 + \Delta \beta_x^2 & 0 \\ \alpha_x\Delta \alpha_x^2 - \beta_x\Delta \beta_x^2 & 0 & \Delta \alpha_x^2 + \Delta \beta_x^2 \end{bmatrix}.$$  \hspace{1cm} (8)$$

Note that for \( \alpha_0 = \beta_0 \) and \( \Delta \alpha_x = \Delta \beta_x \), we obtain the first-order relation \( \Delta q_x^2 = \alpha_x^2\Delta \alpha_x^2 + \beta_x^2\Delta \beta_x^2 \) previously derived by de Jeu et al. (1996). The condition \( \Delta \alpha_x^2 \to 0 \) depends on the beam characteristics and can be realised using synchrotron radiation or variable grating parabolic multilayer optics which produce highly parallel beams. During a diffuse scan, the eigenvector coordinate system rotates in the plane of incidence. In fact, for the case of rocking scans, the eigenvector coordinate system corresponds approximately to the original one because of the geometrical constraint \(|\alpha_0| \leq \theta\). Consequently, we can further simplify the calculation of the intensity in equation (7). One can open the detector slit \( \delta_0 \) widely without modifying the relevant in-plane resolution \( \Delta q_x^2 \) (see §5). In this way, \( \Delta q_x \) is sufficiently large to induce a fast decay of \( \exp(-y^2\Delta q_x^2/2) \). Therefore, only the region \( y \approx 0 \) will contribute to the integral, like in the case of a \( \delta \) function. This allows us to keep in the integrand only \( \langle \rho(0)\rho(x, y = 0, z) \rangle \) and reduces the calculation to a double integration over \( x \) and \( z \) only. In the reciprocal-space representation the resolution function is reduced to a function of \( q_x \) and \( q_z \) only. Information about \( q_y \) is lost as a result of the large smearing in the \( y \) direction, but does not influence the information about \( q_z \). One finally arrives at an expression similar to equation (1):

$$I(q_x, q_z) = \int dq_x' \int dq_z' \mathcal{R}(q_x', q_z') S(q_x - q_x', q_z - q_z'),$$  \hspace{1cm} (11)$$
The mean square deviations with half width at half-maximum, HWHM, measured by $q_x$, the component in the plane of the sample beam, is isotropic in this plane. Note that in the limit $I_{\text{diff}}$ (coincident with $Oxy$), determines the minimal accessible $q_{||}$ range (see also §5). Hence, for liquid systems, the low-$q_{||}$ range can be measured by $q_x$, while the high-$q_{||}$ range is accessible by $q_y$, making it possible to record the fluctuation spectrum from macroscopic down to molecular dimensions.

4. Determination of the dispersion angles

The mean square deviations $\Delta q_x^2$, account for the incident-beam angular dispersion, directly related to the beam divergence, which depends on the optical settings between the X-ray source and the sample. It contributes, together with the beam width due to the pre-sample entrance slits $S_{E_x}$, to the half width at half-maximum, HWHM, of the intensity profile $I(\beta_{i,o})$ measured by a detector scan in or out of the plane of incidence. In such a scan, the angular distribution due to the beam width is a step function of width $\arctan(S_{E_x}/D)$, where $D$ is the distance between the detector and the centre of the diffractometer (coincident with $O$ in Fig. 1). The measured intensity profile $I(\beta_{i,o})$ is convoluted with the detector slits $S_{E_x}$, and depends on $D$:

$$I(\beta_{i,o}) = I_0 \exp(-\beta_{i,o}^2 \ln 2/\text{HWHM}_{i,o}^2) \ast \Pi(\beta_{i,o}),$$

with

$$\Pi(\beta_{i,o}) = \begin{cases} 1 & \text{if } |\beta_{i,o}| \leq \arctan(S_{D_o}/D)/2, \\ 0 & \text{elsewhere}. \end{cases}$$

Assuming Gaussian distributions, we obtain the following relation for the angular mean square deviations of the incident beam:

$$\Delta q_x^2 = \text{HWHM}_{i,o}^2/(2 \ln 2) - \arctan^2(S_{E_x}/D)/12.$$  (14)

The mean square deviations $\Delta \beta_{i,o}^2$ are related to the acceptance solid angle of the detector, which depends both on the illuminated area of the sample and on the detector slits, as shown in Fig. 4. The incident-beam divergence can be used to evaluate the effective footprint $L_{i,o}$ in and out of the plane of incidence, respectively. Two accepting angles, $\beta_{i,o}^{\min}$ and $\beta_{i,o}^{\max}$ define the angular distribution $p$ of the intensity entering the detector aperture. Note that $p$ also describes the intensity profile in the direction $\beta_{i,o}$, collected during a detector scan around $\beta_{i,o}$. An important consequence of this is discussed in §5. For $D \gg \max (L_{i,o} \sin \beta_{i,in}, S_{D_o})$, $p$ has a trapezoidal form with top $2\beta_{i,o}^{\min}$ and base $2\beta_{i,o}^{\max}$. Explicitly, $p$ reads

$$p(\beta_{i,o}) = \begin{cases} 1/(\beta_{i,o}^{\max} + \beta_{i,o}^{\min}) & \text{if } |\beta_{i,o}| < \beta_{i,o}^{\min} \\ (\beta_{i,o}^{\max} - \beta_{i,o}^{\min})/[(\beta_{i,o}^{\max})^2 - (\beta_{i,o}^{\min})^2] & \text{if } \beta_{i,o}^{\min} < |\beta_{i,o}| < \beta_{i,o}^{\max} \\ 0 & \text{if } |\beta_{i,o}| > \beta_{i,o}^{\max}. \end{cases}$$  (15)

We replace this trapezoidal distribution by a Gaussian distribution giving the same mean square values, which leads to

$$\Delta \beta_{i,o}^2 = (1/6)((\beta_{i,o}^{\min})^2 + (\beta_{i,o}^{\max})^2).$$  (16)
and perform the integration over the $xy$ plane in the following way:

$$\int \int dx dy \exp[i(q_x x + q_y y) - (1/2) \Delta q_x^2 - (1/2) \Delta q_y^2] G(q_x, q_y)$$

$$= (1/\Delta q_x \Delta q_y) \int d^2 q \int d_r r_I(q - q') r_I(q) \times \exp[-q_x^2/2\Delta q_x^2 - q_y^2/2\Delta q_y^2] G(q_x, q_y),$$

(21)

where $I_0$ is the Bessel function of order zero. Although this procedure requires an additional integration, it is much more efficient because the range of integration is smaller than in equation (7).

In the case of systems with a finite correlation distance, $G(q_x, q_y)$ would decay exponentially to a constant value $G(q_x, q_y) \propto \exp[-q_x^2/(2\Delta q_x^2)]$. Integration of this constant with $\exp(r_{1f} \cdot q_f)$ provides a delta function. In such a situation there are good reasons to split the total intensity into two parts. The first one is the specular reflectivity due to $G(q_x, q_y)$; the second is the diffuse scattering due to $[G(q_x, q_y) - G(q_x, q_y)]$ in the integrand. The specular reflectivity can be analysed separately using, for example, the matrix formalism of Parrat (1954). To carry out this type of analysis one has to subtract the diffuse contribution to the specular signal which arises because of the finite size of the detector aperture. This requires the resolution treatment to be modified accordingly (Shindler & Suter, 1992).

In the case of smectic liquid crystals, the situation is different because the mean square displacement fluctuations diverge due to Landau–Peierls instability (e.g., de Gennes & Prost, 1993; Vertogen & De Jeu, 1988). Therefore, no correlation distance can be identified to which the height–height correlation function $G(q_x, q_y)$ decays: the function $\langle [u_{m}(0) - u_{n}(r)]^2 \rangle$ tends formally to zero as $r_1$ increases. As a result, $G$ decays algebraically to zero and we face the following features. In the first place, there is no basis to split the intensity into two parts. Secondly, the integral in equation (18) diverges and only the convolution with the resolution function makes it finite. Consequently, the accessible range for the fluctuation spectrum depends on the parametrization of the resolution function.

Let us now analyse the combined effect of the resolution and correlation functions on the scattered intensity in the cases of diffuse scans in and out of the plane of incidence, where $I(q_f)$ is probed as described in §3. The major effect of the resolution is to limit the flux of scattered intensity in the detector and to broaden the structural details in $I(q_f)$. In the case of thin films, the main signature of structural details comes from the Fresnel factor $R_{q}(q_f)$ in equation (18) and results in interference fringes, called Kiessig fringes (Born & Wolf, 1980). For a detector scan in the plane of incidence, $q_y$ is varied and the Kiessig fringes are smeared out by the resolution. For diffuse scans out of the plane of incidence, $q_y$ is kept constant and the resolution has no smearing effects. Another important feature is related to the distinction between specular and off-specular dominated regions. One may define a specular region $I_{\text{spec}}(q_f) = I(q_f) \approx 0$ corresponding to a certain positional range of the detector in the domain of the specularly reflected beam sheet. As already mentioned in §4, $\Delta q_y^2$ corresponds to the mean square...
deviation of the intensity distribution \( I(q_{||}) \) collected by a
detector scan around \( q_{||} \) (see Fig. 4). Therefore, the region
corresponding to \( 0 \lesssim q_{||} \lesssim \Delta q_{||} \) is dominated by the specularly
reflected intensity. In particular, this may provide a method to
subtract the pure diffuse scattering from the totally reflected
intensity. The diffuse region is influenced both by the resolution
and the correlation function. More precisely, the correlation
function influences the slope of the diffuse scattering in
different manners depending on the type of resolution and
geometry used. As a result, beyond the ‘plateau region’, the
in-plane resolution factor in equation (21) has no effect on the
shape of the scattering. Thus, there exists an intermediate \( q_{||} \)
region where the logarithmic term in \( g(r_{ij}) \) is dominant (in
between the ‘plateau’ and high \( q_{||} \) regions). In this region, the
intensity follows an algebraic decay law of the following type:

\[
I(q_{||}) \sim \int dq_{||} \exp(i\mathbf{q}_{||} \cdot \mathbf{r}_{ij})r_{ij}^{-\eta} \sim q_{||}^{-D+\eta},
\tag{22}
\]

where \( D = 1 \) or \( 2 \), depending on whether a one- or
two-dimensional integration is performed. At higher \( q_{||} \) regions, we
expect a nonlinear deviation from the algebraic decay to be
induced by the bending elasticity modulus \( K \).

Let us now check the points raised in the above discussion
using some concrete examples. Fig. 5 shows calculations of the
scattering in or out of the plane of incidence from a smectic
film computed with the same physical parameters \( (\gamma, K, d, N) \)
used in \( G(q_{||}, r_{ij}) \) above. The left curves are rocking scans using
one- or two-dimensional integration [performed with or
without detector slit \( S_{D_{||}} \), respectively] and using the covari-
ance matrix (8). The right curve is a detector scan out of the
plane of incidence using necessarily a two-dimensional inte-
gration and the covariance matrix (11). All the curves exhibit a
large ‘plateau’ region at low \( q_{||} \) distinct from a smooth negative
slope starting at \( q_{||} \simeq \Delta q_{||} \). As explained above, the first part
can be associated with the specularly reflected intensity and
the second part with the off-specular intensity. The slope
behaviour of the diffuse part is clearly dominated by the
correlation function. Indeed, there are large intermediate
regions having slopes either close to \( q_{||}^{1+\eta} \) for a rocking scan
without detector slit \( S_{D_{||}} \) (left solid line), or close to \( q_{||}^{2+\eta} \) for a
diffuse scan out of the plane of incidence (right solid line) as a
result of the dimensionality of the integration in equation (22).
The effect of the bending elasticity modulus \( K \) occurs at higher
\( q_{||} \) and results in a strong nonlinear attenuation of the diffuse
intensity, as can be seen in detector scans out of the plane of
incidence (right solid line). Note that for rocking scans it is
difficult to reach sufficiently high values of \( q_{||} \) to see this effect
because of the geometrical constraints (see Fig. 2).

Finally, we note that the interplay between resolution and
correlation functions can change in a subtle way depending on
the geometry of the experiment. This is illustrated Fig. 5 for
the rocking scan upon introducing a finite vertical detector slit
\( S_{D_{||}} \) (see left dashed line). In this case, a two-dimensional
integration is performed as in equation (21). However,
because \( q_{||} = 0 \) for a rocking scan, a slope regime between
\( q_{||}^{1+\eta} \) and \( q_{||}^{2+\eta} \) is obtained. Note that the shape of the
‘plateau’ region remains unchanged upon addition of \( S_{D_{||}} \)
because the relevant in-plane resolution component \( \Delta q_{||}^{2} \)
does not depend on \( \Delta q_{||}^{2} \).

When one wishes to extract information from the off-
specular scattering, it can be useful to adjust the resolution in
order to obtain a minimal size of the ‘plateau’ region and a
maximal flux of diffuse intensity in the detector. The first
condition is fulfilled by minimizing the value of \( \Delta q_{||}^{2} \),
which means using a rather parallel beam with relatively narrow
detector slits in the direction of scanning. Furthermore,
specific conditions depend on the geometry of the experiment,
in particular on the type of correlations between the resolution
components \( \Delta q_{||}^{2}, \Delta q_{||}^{2} \) and \( \Delta q_{||}^{2} \), as already discussed in
section §3. In the case of diffuse scans in the plane of inci-
dence, the relevant in-plane resolution \( \Delta q_{||}^{2} \) does not change
when \( \Delta q_{||}^{2} \) is varied. Therefore, it is a good strategy to open the
vertical detector slit \( S_{D_{||}} \) widely to increase the flux of intensity
in the detector without loosing the relevant in-plane resolution
\( \Delta q_{||}^{2} \). In the case of diffuse scans out of the plane of
incidence, \( \Delta q_{||}^{2} \) and \( \Delta q_{||}^{2} \) are correlated. However, in this
geometry, the vertical resolution \( \Delta q_{||}^{2} \) does not depend on the
in-plane resolution. Therefore, it is an interesting strategy to
open the horizontal slit \( S_{D_{||}} \) widely to increase the flux in the
detector without loosing the resolution \( \Delta q_{||}^{2} \) corresponding to
the high-\( q_{||} \) range probed.

6. Conclusion

We have given a comprehensive description of the resolution
function in the context of grazing-angle X-ray scattering
experiments. We have shown how to calculate the resolution
function \( R \) and have given explicit expressions relating the
mean square deviations of \( q \) and of the relevant direct-space
angles for some common scattering configurations. For these
scattering geometries, we have used the formalism given to calculate the scattering from free-standing smectic films in order to analyse the shape of the scattered intensity $I(q_{||})$. In particular, we have defined two regions, a 'plateau' region for $q_{||} < \Delta q_{||}$, which can be associated with the specularly reflected intensity, and a purely diffuse region for $q_{||} \geq \Delta q_{||}$, in which we have described the combined influence of the correlation and the resolution functions for each scanning geometry.

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**References**


