Grazing-incidence small-angle X-ray scattering (GISAXS) on small periodic targets using large beams

Mika Pflüger, Victor Soltwisch, Jürgen Probst, Frank Scholze and Michael Krumrey
1 Background Correction

In order to extract the scattering of the targets only, the background $B$ was fitted for each measurement, assuming that the background $B$ can be factorized to $B(\alpha_f, \theta_f) = A(\alpha_f) \cdot T(\theta_f)$. This factorization is motivated by the assumption that $T(\theta_f)$ depends mainly on the correlations of the roughness of the substrate in $x$- and $y$-direction, which in small-angle approximation does not depend on $\alpha_f$. For the function $A(\alpha_f)$, a smooth B-spline approximation of degree 2 was used to closely follow the scattering of the background around the critical angle of total external reflection $\alpha_c$ of the substrate (see fig. 1 a)). In order to only fit the substrate contribution, a cut along $\alpha_f$ was taken between the first and second grating diffraction orders. For the function $T(\theta_f)$, a polynomial of degree 4 was fitted to a cut along $\theta_f$ at $\alpha_f > 0.8^\circ$, i.e.
above the sample scattering features (see fig. 1 b)). The resulting smooth background was subtracted from the GISAXS measurement, yielding the scattering from the target only (fig. 2).

![GISAXS scattering](image)

**Figure 2**: GISAXS scattering of smallest target, a) raw data b) after background subtraction. The background subtraction works well above the critical angle of the substrate $\alpha_c$, but fails below $\alpha_c$.

2 Position of Grating Diffraction Orders in GISAXS in Sample Coordinates

2.1 Coordinate System and Ewald Sphere

We use a coordinate system where the $x$-$y$-plane is the sample plane, with the $x$-axis the intersection of the scattering plane with the sample plane and the $y$-axis perpendicular to the $x$-axis. The $z$-axis is the normal of the sample plane. The $k$-space is the reciprocal of the real space, with the corresponding axes in the same direction as the real axes. In this space, the wavevectors of the incoming beam $k_i$ and the scattered beam $k_f$ are

$$k_i = k_0 \begin{pmatrix} \cos \alpha_i \\ 0 \\ -\sin \alpha_i \end{pmatrix}$$  \hspace{1cm} (1)

$$k_f = k_0 \begin{pmatrix} \cos \alpha_f \cos \theta_f \\ \cos \alpha_f \sin \theta_f \\ \sin \alpha_f \end{pmatrix}$$  \hspace{1cm} (2)

$$k_0 = |k_i| = |k_f| = \frac{2\pi}{\lambda}$$  \hspace{1cm} (3)

with the incident angle $\alpha_i$, the angle between the sample plane and the scattered beam $\alpha_f$ and the angle between the projection of the scattered beam on the sample plane and the $x$-axis $\theta_f$. 
as well as the incident wavelength \( \lambda \).

We define the scattering vector \( \mathbf{q} = \mathbf{k}_f - \mathbf{k}_i \), which expressed in angle coordinates is

\[
\mathbf{q} = k_0 \begin{pmatrix} \cos \alpha_f \cos \theta_f - \cos \alpha_i \\ \cos \alpha_f \sin \theta_f \\ \sin \alpha_f + \sin \alpha_i \end{pmatrix},
\]

(4)
together with (3) we can write the equation for the Ewald sphere of elastic scattering

\[
k_0 = |\mathbf{k}_f| = |\mathbf{q} + \mathbf{k}_i|
\]

(5)
\[
\Rightarrow k_0^2 = |\mathbf{q} + \mathbf{k}_i|^2 = (q_x + k_{i,x})^2 + (q_y + k_{i,y})^2 + (q_z + k_{i,z})^2
\]

(6)

\[= (q_x + k_0 \cos \alpha_i)^2 + q_y^2 + (q_z - k_0 \sin \alpha_i)^2. \]

2.2 Perfectly Aligned Grating

The perfectly aligned grating has infinite grating lines parallel to the \( x \)-axis, which lie in the sample plane and are separated by the pitch \( p \). The reciprocal space representation of the perfectly aligned grating comprises grating truncation rods (GTR), which are parallel to the \( q_z \)-axis in the \( q_z \)-\( q_y \)-plane and separated by \( 2\pi / p \) in \( q_y \):

\[q_x = 0\]
\[q_y = n 2\pi / p = k_0 n \lambda / p\]

with the grating diffraction order \( n \in \mathbb{Z} \). The intersection of the Ewald sphere (6) with the GTR yields

\[
k_0^2 = (0 + k_0 \cos \alpha_i)^2 + (n k_0 \lambda / p)^2 + (q_z - k_0 \sin \alpha_i)^2
\]

(9)
solving for \( q_z \)

\[
(q_z - k_0 \sin \alpha_i)^2 = k_0^2 (1 - \cos^2 \alpha_i) - (n k_0 \lambda / p)^2
\]

(10)
\[
= k_0^2 (\sin^2 \alpha_i - (n \lambda / p)^2)
\]

\[
\Rightarrow q_z = k_0 \left( \sin \alpha_i \pm \sqrt{\sin^2 \alpha_i - (n \lambda / p)^2} \right)
\]

(11)
discarding the solution with the minus as it corresponds to reflections below the sample horizon

\[q_z = k_0 \left( \sin \alpha_i + \sqrt{\sin^2 \alpha_i - (n \lambda / p)^2} \right). \]

To summarize:

\[
\mathbf{q}_{\text{grating, aligned}} = k_0 \begin{pmatrix} 0 \\ n \lambda / p \\ \sin \alpha_i + \sqrt{\sin^2 \alpha_i - (n \lambda / p)^2} \end{pmatrix}.
\]

(13)
To express the scattering in angle coordinates, we use (4), (7), (8) and (12), giving

\[ q_z : \sin \alpha_f + \sin \alpha_i = \sin \alpha_i \left( 1 + \sqrt{1 - \left( \frac{n \lambda}{p \sin \alpha_i} \right)^2} \right) \]

\[ \Rightarrow \alpha_f = \arcsin \left( \sqrt{\sin^2 \alpha_i - \left( \frac{n \lambda}{p} \right)^2} \right) \] (14)

\[ q_y : \cos \alpha_f \sin \theta_f = \frac{n \lambda}{p} \]

\[ \Rightarrow \sin \theta_f = \frac{n \lambda}{p \cos \alpha_f} \] (15)

\[ q_x : \cos \alpha_f \cos \theta_f - \cos \alpha_i = 0 \]

\[ \Rightarrow \cos \theta_f = \frac{\cos \alpha_i}{\cos \alpha_f} \] (16)

\[ \frac{q_y}{q_x} : \tan \theta_f = \frac{\sin \theta_f}{\cos \theta_f} = \frac{n \lambda}{p \cos \alpha_f} \]

\[ \Rightarrow \theta_f = \arctan \left( \frac{n \lambda}{p \cos \alpha_i} \right) \] (17)

### 2.3 Misaligned Grating

For the misaligned grating, the grating lines are rotated around the \( z \)-axis by \( \varphi \), and thus the GTRs are also rotated around the \( k_z \)-axis by \( \varphi \), giving the conditions

\[ q_x = k_0 \sin \varphi \frac{n \lambda}{p} \]

\[ q_y = k_0 \cos \varphi \frac{n \lambda}{p} \] (18)

The intersection with the Ewald sphere (6) now yields

\[ k_0^2 = (k_0 \sin \varphi \frac{n \lambda}{p} + k_0 \cos \alpha_i)^2 + (k_0 \cos \varphi \frac{n \lambda}{p} )^2 + (q_z - k_0 \sin \alpha_i)^2 \]

\[ = k_0^2 \left( (\sin^2 \varphi + \cos^2 \varphi)(\frac{n \lambda}{p})^2 + 2 \sin \varphi \cos \alpha_i \frac{n \lambda}{p} + \cos^2 \alpha_i \right) + (q_z - k_0 \sin \alpha_i)^2 \] (20)

solving for \( q_z \)

\[ (q_z - k_0 \sin \alpha_i)^2 = k_0^2 \left( 1 - \cos^2 \alpha_i - (\frac{n \lambda}{p})^2 - 2 \sin \varphi \cos \alpha_i \frac{n \lambda}{p} \right) \]

\[ = k_0^2 \left( \sin^2 \alpha_i - (\frac{n \lambda}{p})^2 - 2 \sin \varphi \cos \alpha_i \frac{n \lambda}{p} \right) \] (21)

\[ \Rightarrow q_z = k_0 \left( \sin \alpha_i \pm \sqrt{\sin^2 \alpha_i - (\frac{n \lambda}{p})^2 - 2 \sin \varphi \cos \alpha_i \frac{n \lambda}{p}} \right) \]

\[ \text{discarding the solution with the minus as it corresponds to reflections below the sample horizon} \]

\[ q_z = k_0 \left( \sin \alpha_i + \sqrt{\sin^2 \alpha_i - (\frac{n \lambda}{p})^2 - 2 \sin \varphi \cos \alpha_i \frac{n \lambda}{p}} \right) \] . (22)
To summarize:

\[ q_{\text{grating}} = k_0 \begin{pmatrix} \frac{\sin \varphi n \lambda / p}{\cos \varphi n \lambda / p} \\ \sin \alpha_i + \sqrt{\sin^2 \alpha_i - (n \lambda / p)^2 - 2 \sin \varphi \cos \alpha_i n \lambda / p} \end{pmatrix} \] . \quad (24)

To express the scattering in angle coordinates, we use (4), (18), (19) and (23), giving

\[ q_z : \quad \sin \alpha_f + \sin \alpha_i = \sin \alpha_i + \sqrt{\sin^2 \alpha_i - (n \lambda / p)^2 - 2 \sin \varphi \cos \alpha_i n \lambda / p} \]
\[ \Rightarrow \alpha_f = \arcsin \left( \sqrt{\sin^2 \alpha_i - (n \lambda / p)^2 - 2 \sin \varphi \cos \alpha_i n \lambda / p} \right) \] \quad (25)

\[ q_y : \quad \cos \alpha_f \sin \theta_f = \cos \varphi n \lambda / p \]
\[ \Rightarrow \sin \theta_f = \frac{\cos \varphi n \lambda / p}{\cos \alpha_f} \] \quad (26)

\[ q_x : \quad \cos \alpha_f \cos \theta_f - \cos \alpha_i = \sin \varphi n \lambda / p \]
\[ \Rightarrow \cos \theta_f = \frac{\sin \varphi n \lambda / p + \cos \alpha_i}{\cos \alpha_f} \] \quad (27)

\[ \frac{q_y}{q_x} : \quad \tan \theta_f = \frac{\sin \theta_f}{\cos \theta_f} = \frac{\cos \varphi n \lambda / p}{\sin \varphi n \lambda / p + \cos \alpha_i} \]
\[ \Rightarrow \theta_f = \arctan \left( \frac{\cos \varphi n \lambda / p}{\sin \varphi n \lambda / p + \cos \alpha_i} \right) \] . \quad (28)